Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Porphyrin-based multi-signal chemosensors for Pb^{2+} and Cu^{2+}

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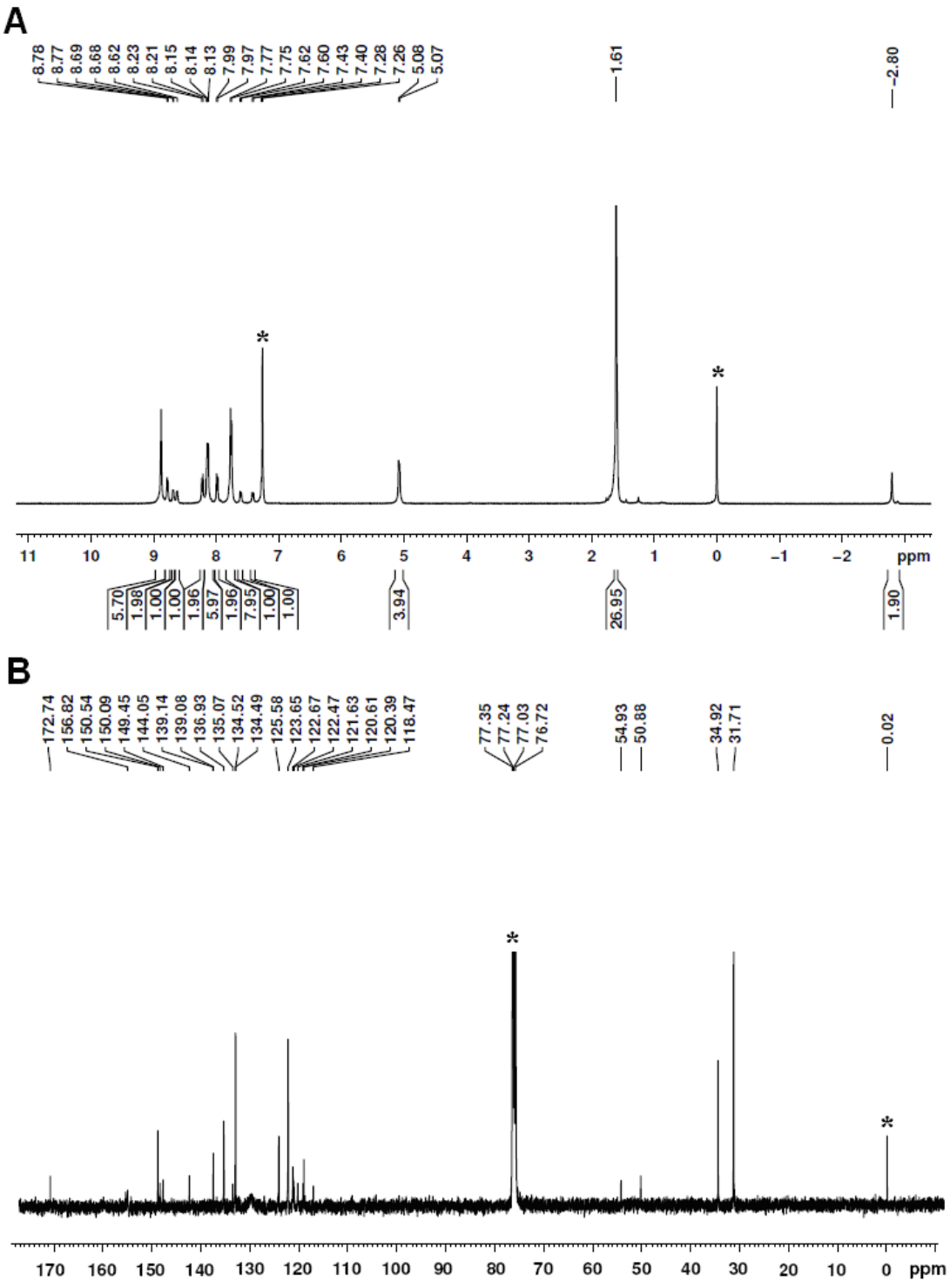

Figure S1. ^{1}H NMR (A) and ^{13}C NMR spectra (B) of Porphyrin-1-DPA **1** in $CDCl_3$. * indicate the residual solvent signals.

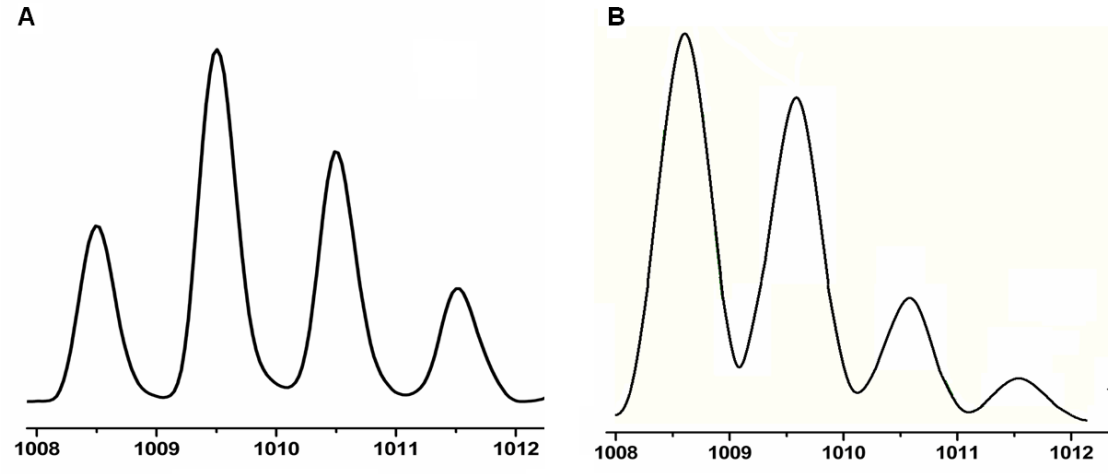

Figure S2. (A) Experimental and (B) simulated isotopic pattern for molecular ion of porphyrin-1-DPA **1** shown in the MALDI-TOF mass spectrum, respectively.

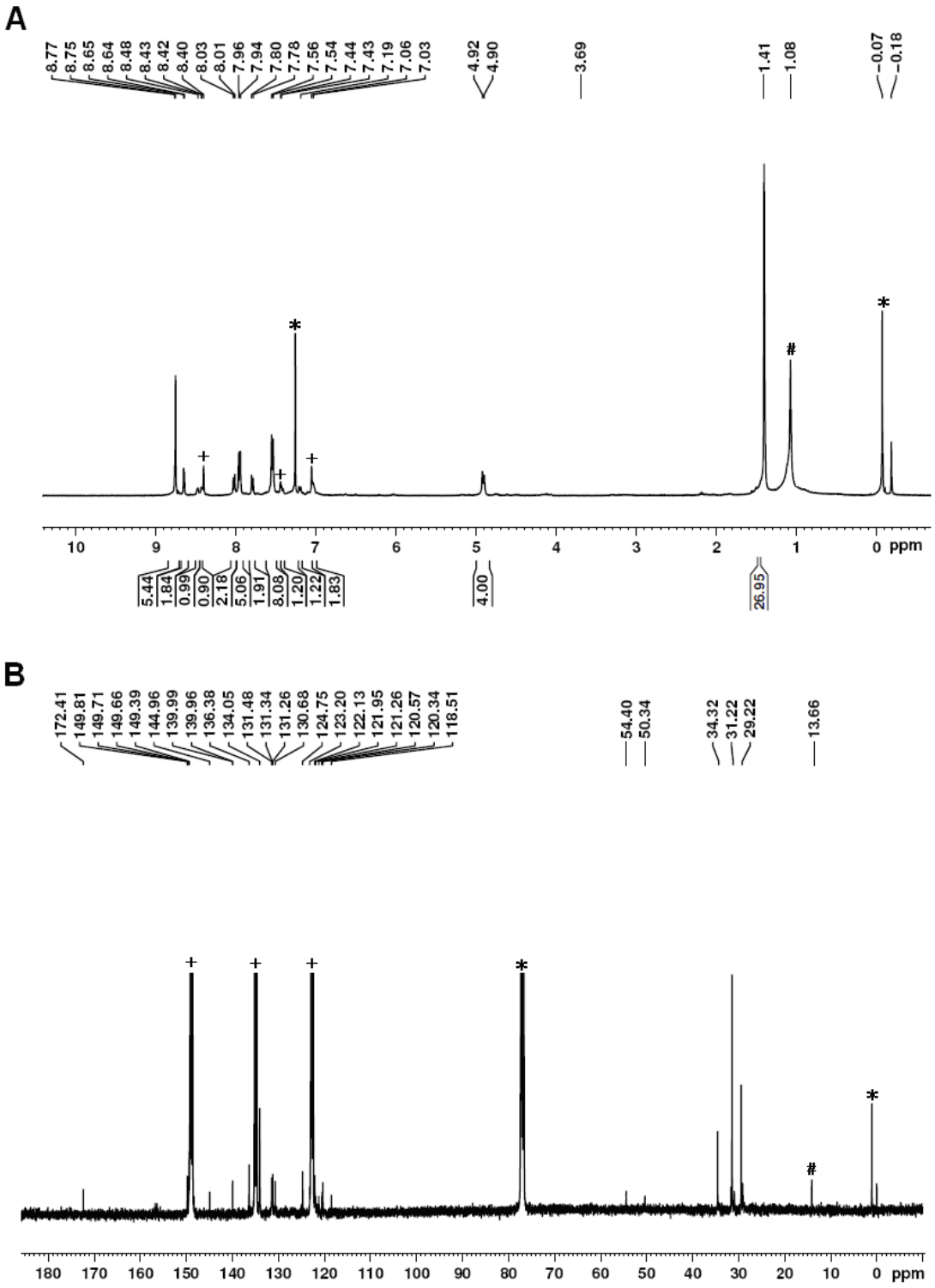

Figure S3. ^{1}H NMR (A) and ^{13}C NMR spectra (B) of **1Zn** in $CDCl_3$/[D_5]Pyridine (9:1). *****, $^{+}$, and # indicate the residual solvent signals of $CHCl_3$, Pyridine, and hexane impurities, respectively.

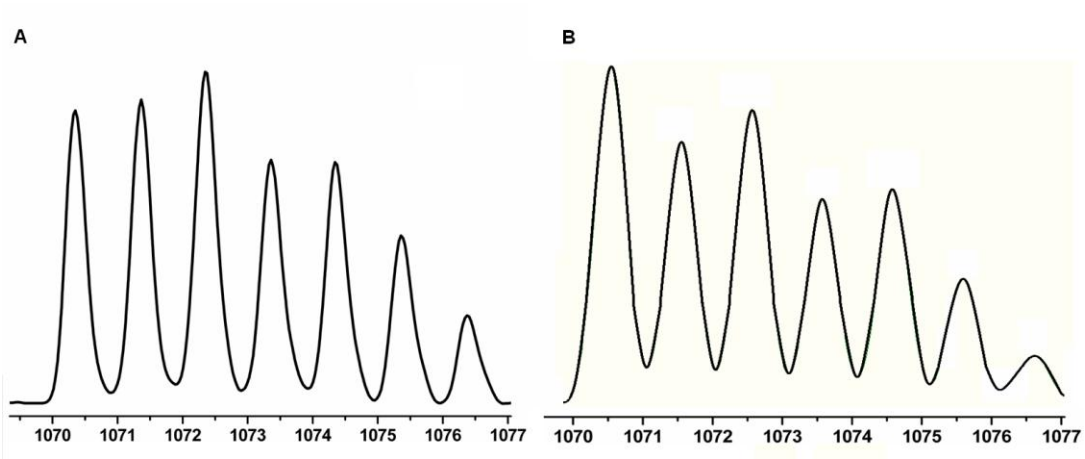

Figure S4. (A) Experimental and (B) simulated isotopic pattern for molecular ion of porphyrin-1-DPA **1Zn** shown in the MALDI-TOF mass spectrum, respectively.

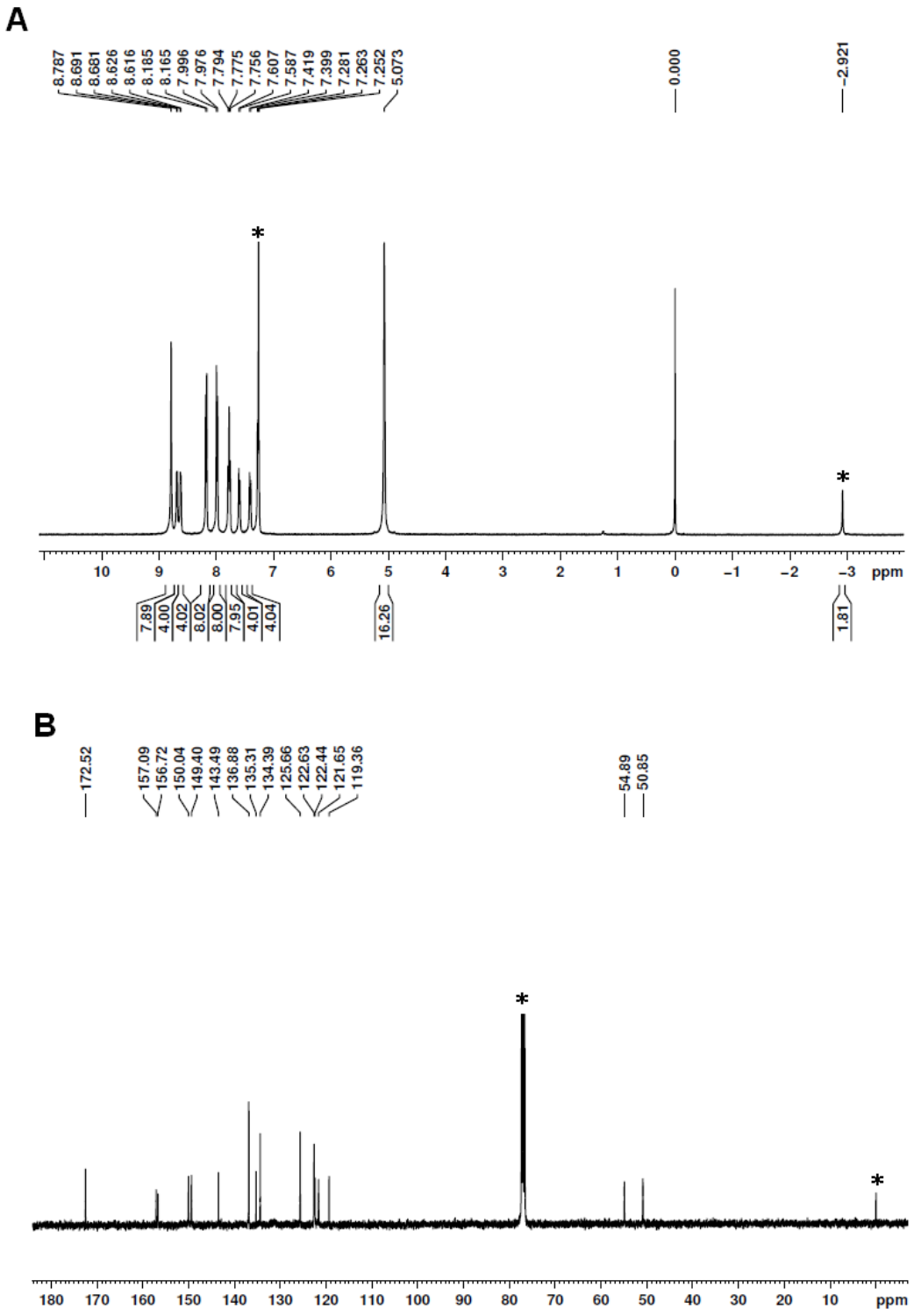

Figure S5. ^{1}H NMR (A) and ^{13}C NMR spectra (B) of Porphyrin-4-DPA **2** in $CDCl_3$. * indicate the residual solvent signals.

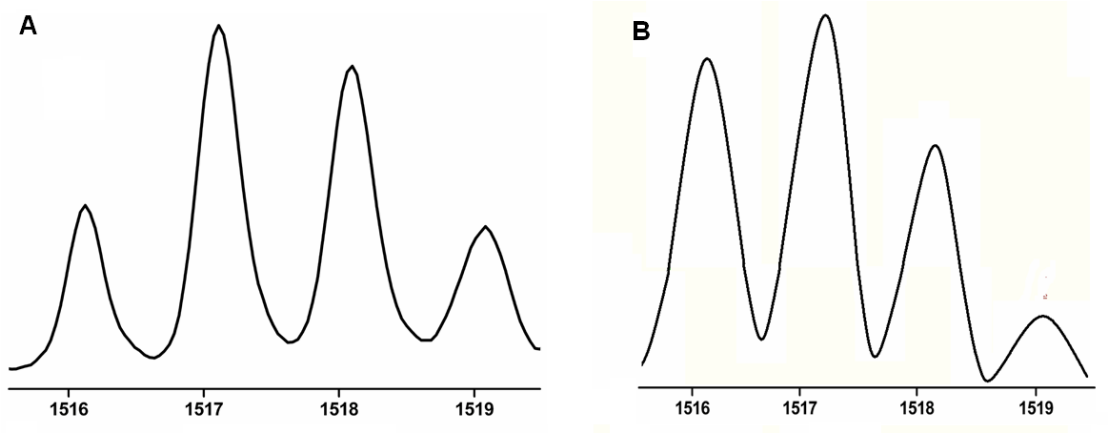

Figure S6. (A) Experimental and (B) simulated isotopic pattern for molecular ion of porphyrin-4-DPA **2** shown in the MALDI-TOF mass spectrum, respectively.

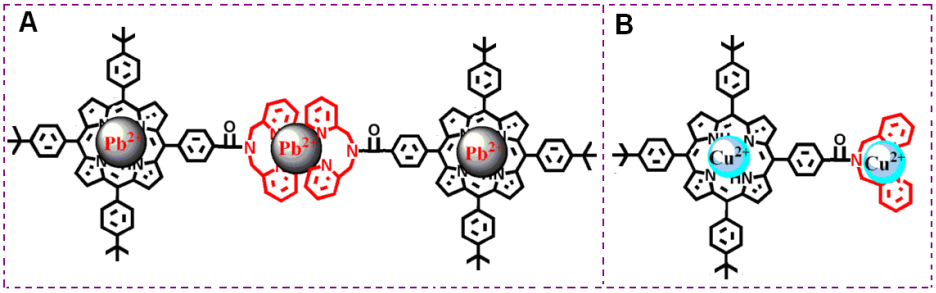

Figure S7. The proposed coordinating mode of porphyrin-1-DPA (**1**) with Pb^{2+} (A) and Cu^{2+} (B), respectively.

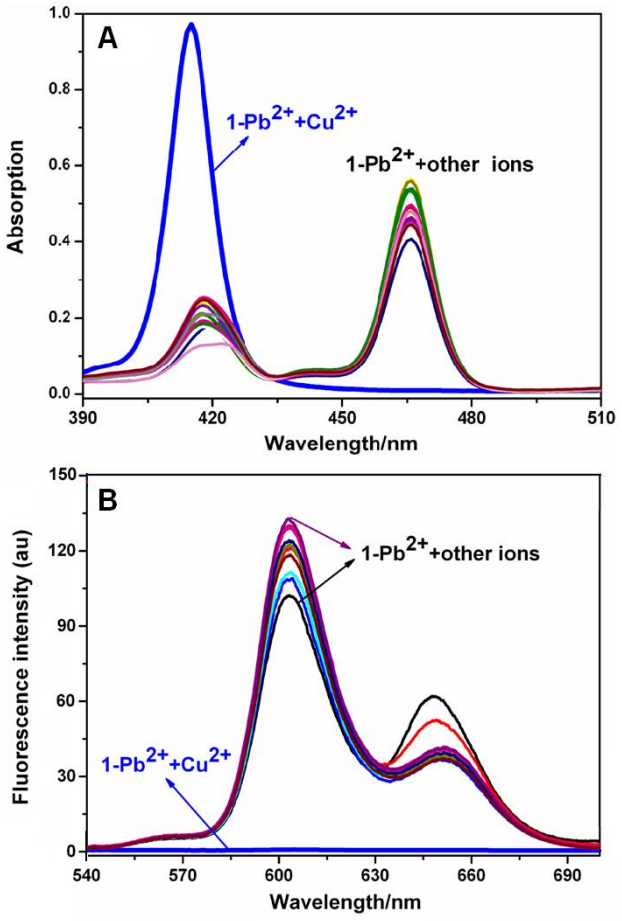

Figure S8. The electronic absorption (A) and fluorescence emission spectra (B) of **1-Pb^{2+}** in CH_2Cl_2/MeOH (1:1) upon addition of K^+, Li^+, Cd^{2+}, Ni^{2+}, Mn^{2+}, Ba^{2+}, Fe^{2+}, Co^{2+}, Mg^{2+}, Ca^{2+}, Na^+, Hg^{2+}, Cu^{2+}, or Zn^{2+} (Pb^{2+}:M = 1:1), respectively, with the excitation of 420 nm.

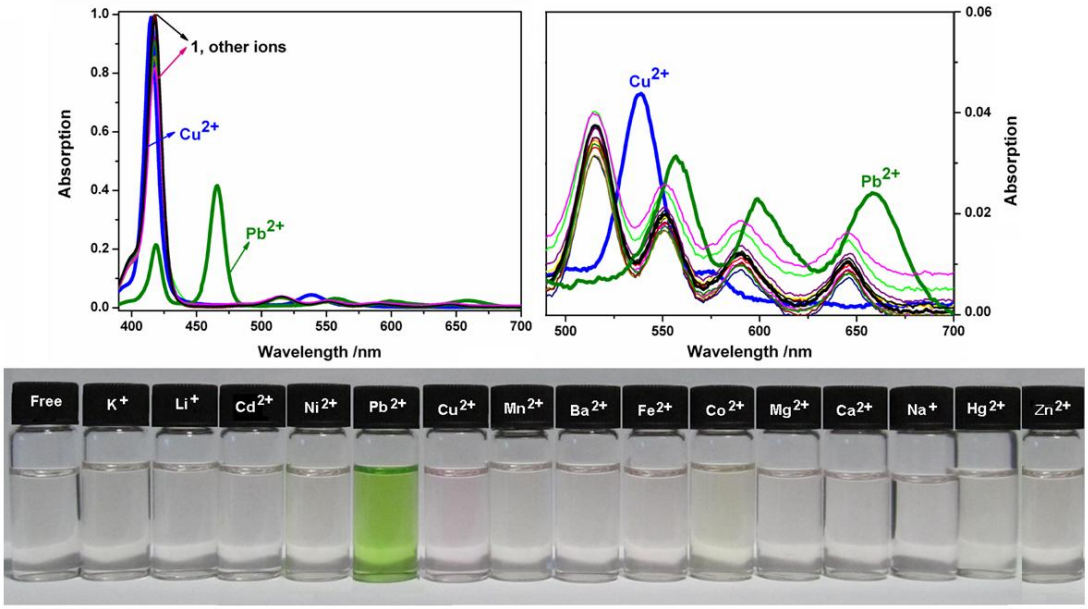

Figure S9. The electronic absorption spectra (top) and the naked color change in solution (bottom) of porphyrin-1-DPA (**1**) (2 μM) in CH_2Cl_2/MeOH (1:1) upon addition of K^+, Li^+, Cd^{2+}, Ni^{2+}, Pb^{2+}, Cu^{2+}, Mn^{2+}, Ba^{2+}, Fe^{2+}, Co^{2+}, Mg^{2+}, Ca^{2+}, Na^+, Hg^{2+}, or Zn^{2+} (10 equiv), respectively.

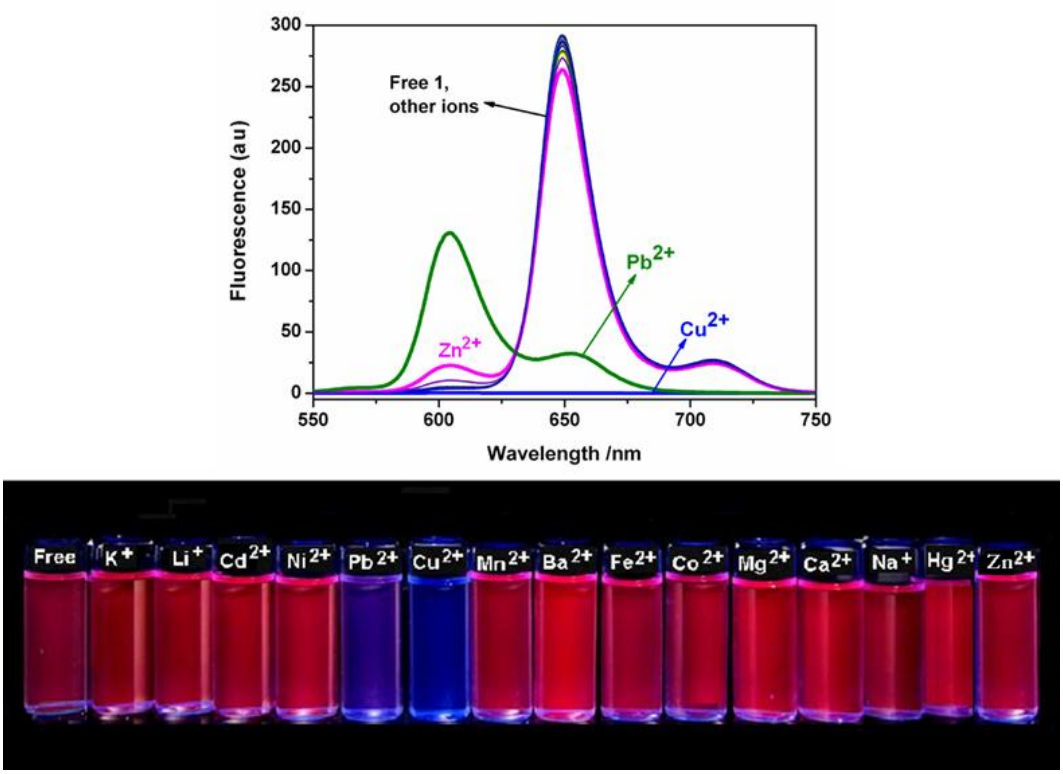

Figure S10. The fluorescence spectra of porphyrin-1-DPA (**1**) (2 μM) in CH_2Cl_2/MeOH (1:1) upon addition of K^+, Li^+, Cd^{2+}, Ni^{2+}, Pb^{2+}, Cu^{2+}, Mn^{2+}, Ba^{2+}, Fe^{2+}, Co^{2+}, Mg^{2+}, Ca^{2+}, Na^+, Hg^{2+}, or Zn^{2+} (10 equiv), respectively, with the excitation of 420 nm.

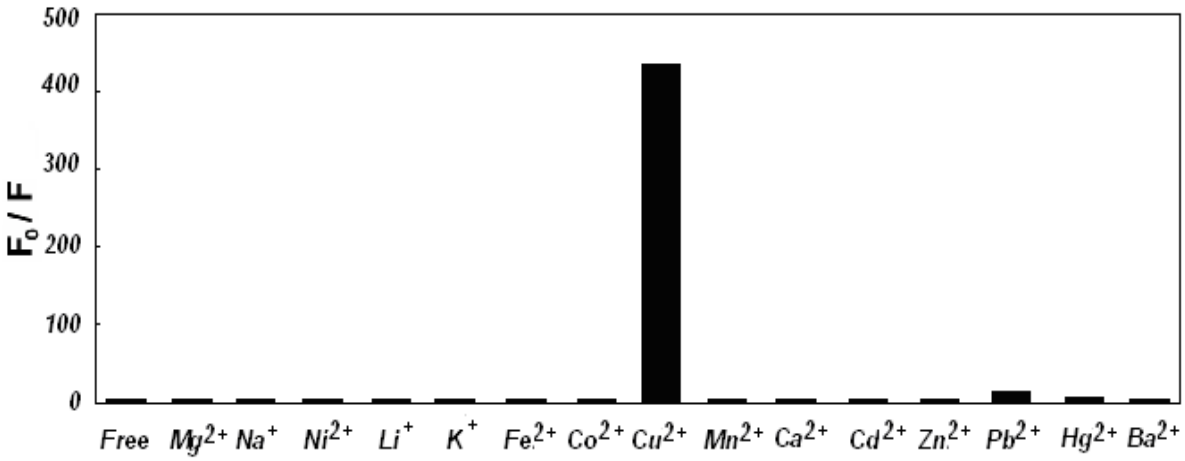

Figure S11. Fluorescence responses of porphyrin-1-DPA (**1)** (2 μM) to various metal cations (10 equiv) in CH_2Cl_2/MeOH (1:1), with the excitation of 420 nm. F_0 and F represent the fluorescence intensity in the range from 620 to 750 nm before and after addition of K^+, Li^+, Cd^{2+}, Ni^{2+}, Pb^{2+}, Cu^{2+}, Mn^{2+}, Ba^{2+}, Fe^{2+}, Co^{2+}, Mg^{2+}, Ca^{2+}, Na^+, Hg^{2+} or Zn^{2+}, respectively.

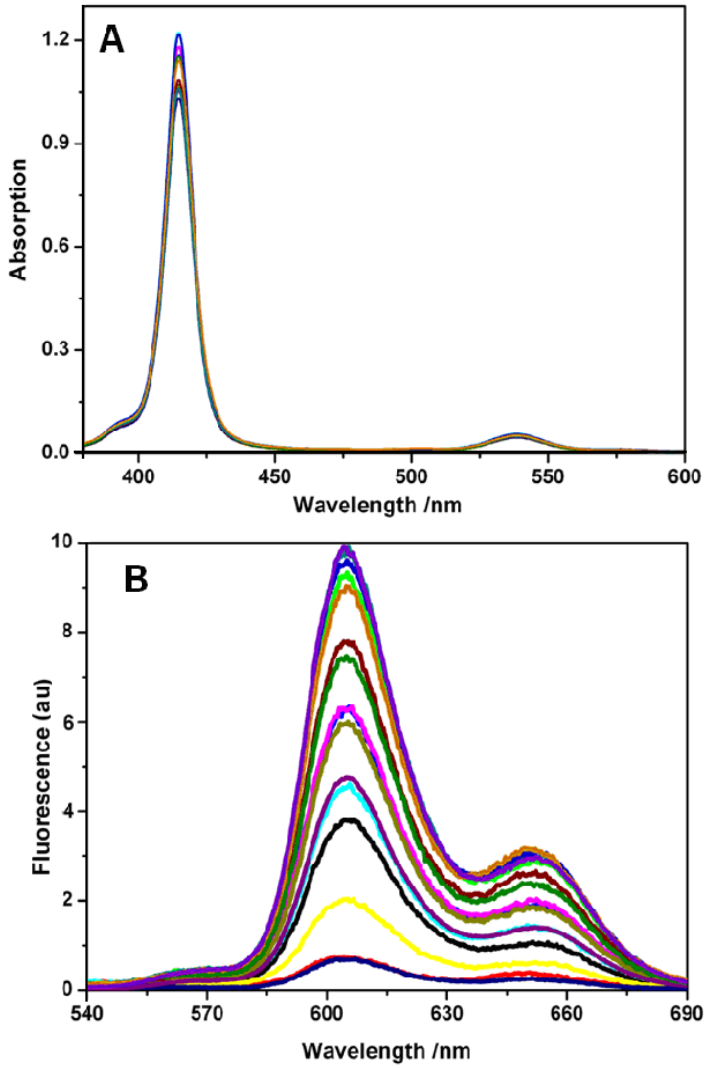

Figure S12. The electronic absorption (A) and fluorescence emission spectra (B) of **1-Cu^{2+}**(10 equiv) in CH_2Cl_2/MeOH (1:1) upon addition of K^+, Li^+, Cd^{2+}, Ni^{2+}, Mn^{2+}, Ba^{2+}, Fe^{2+}, Co^{2+}, Mg^{2+}, Ca^{2+}, Na^+, Hg^{2+}, Pb^{2+}, or Zn^{2+} (10 equiv), respectively, with the excitation of 420 nm.

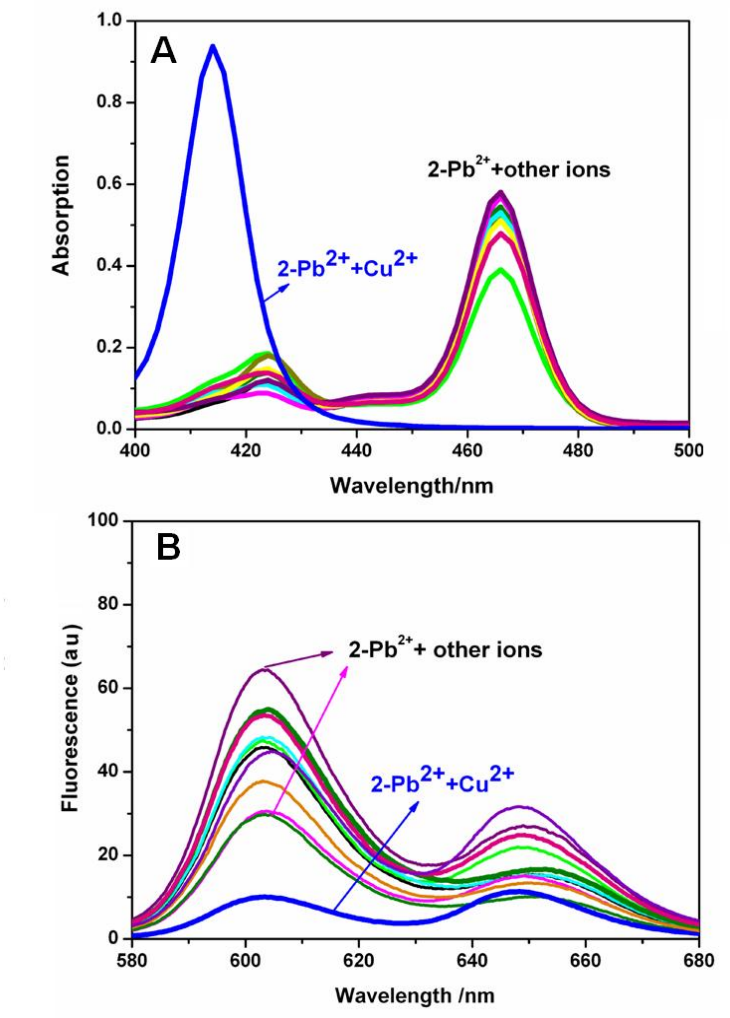

Figure S13. The electronic absorption (A) and fluorescence emission spectra (B) of **2-Pb^{2+}** in CH_2Cl_2/MeOH (1:1) upon addition of Fe^{2+}, Co^{2+}, Hg^{2+}, Mn^{2+}, Zn^{2+}, Ni^{2+}, Cd^{2+}, Ca^{2+}, Ba^{2+}, Mg^{2+}, Li^{+}, Na^{+}, Cu^{2+}, or K^{+} (Pb^{2+}:M = 1:1), respectively, with the excitation of 420 nm.

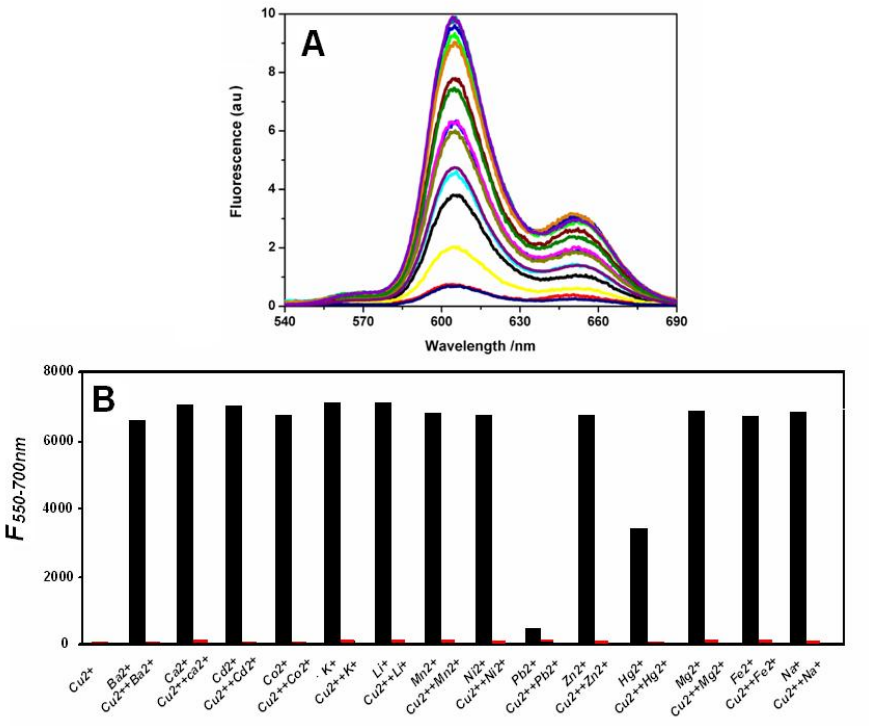

Figure S14. The fluorescence emission spectra (A) and the change of fluorescence intensity in the range from 550 to 700 nm (B) of **2-Cu^{2+}** in CH_2Cl_2/MeOH (1:1) upon addition of Fe^{2+}, Co^{2+}, Hg^{2+}, Mn^{2+}, Zn^{2+}, Ni^{2+}, Cd^{2+}, Ca^{2+}, Ba^{2+}, Mg^{2+}, Li^{+}, Na^{+}, Pb^{2+}, or K^{+} (Cu^{2+}:M = 1:1), respectively, with the excitation of 420 nm.

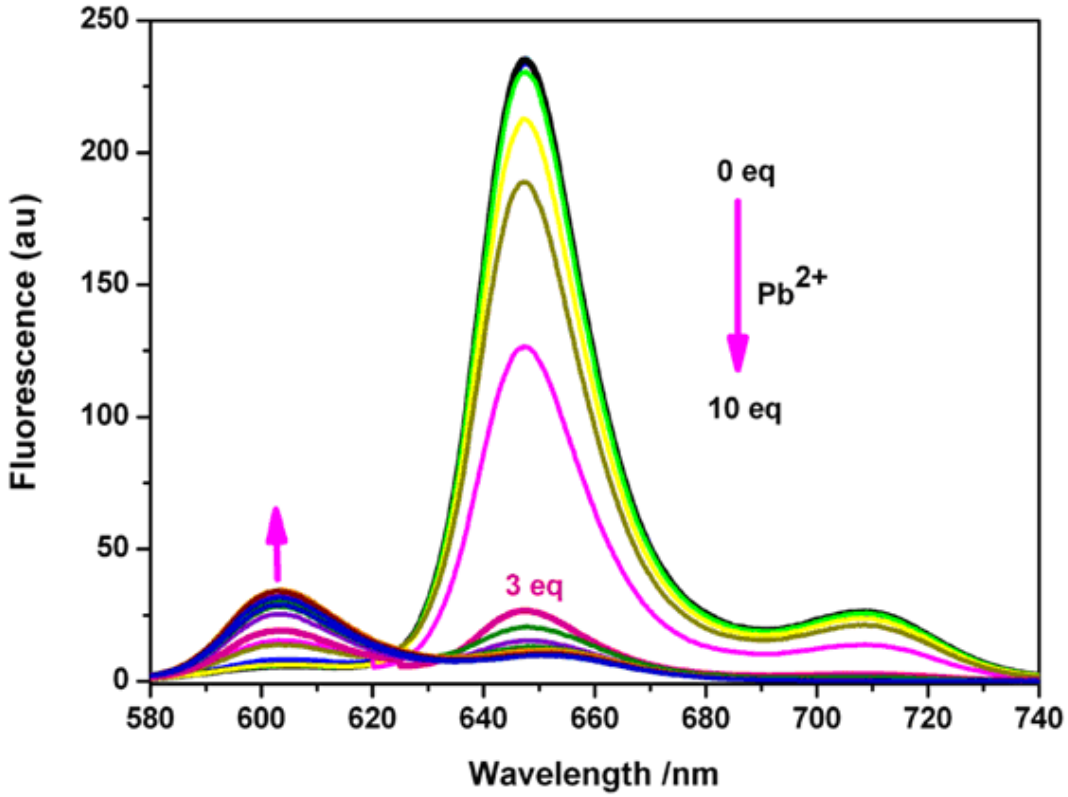

Figure S15. The fluorescent emission spectra of porphyrin-4-DPA (**2**) (2 μM) in CH_2Cl_2/MeOH (1:1) upon addition of increasing amount (0, 0.4, 0.8, 1, 1.2, 1.4, 1.6, 2, 2.5, 3, 4, 6, 8 and 10 equiv) of Pb^{2+}, respectively, with the excitation of 420 nm.

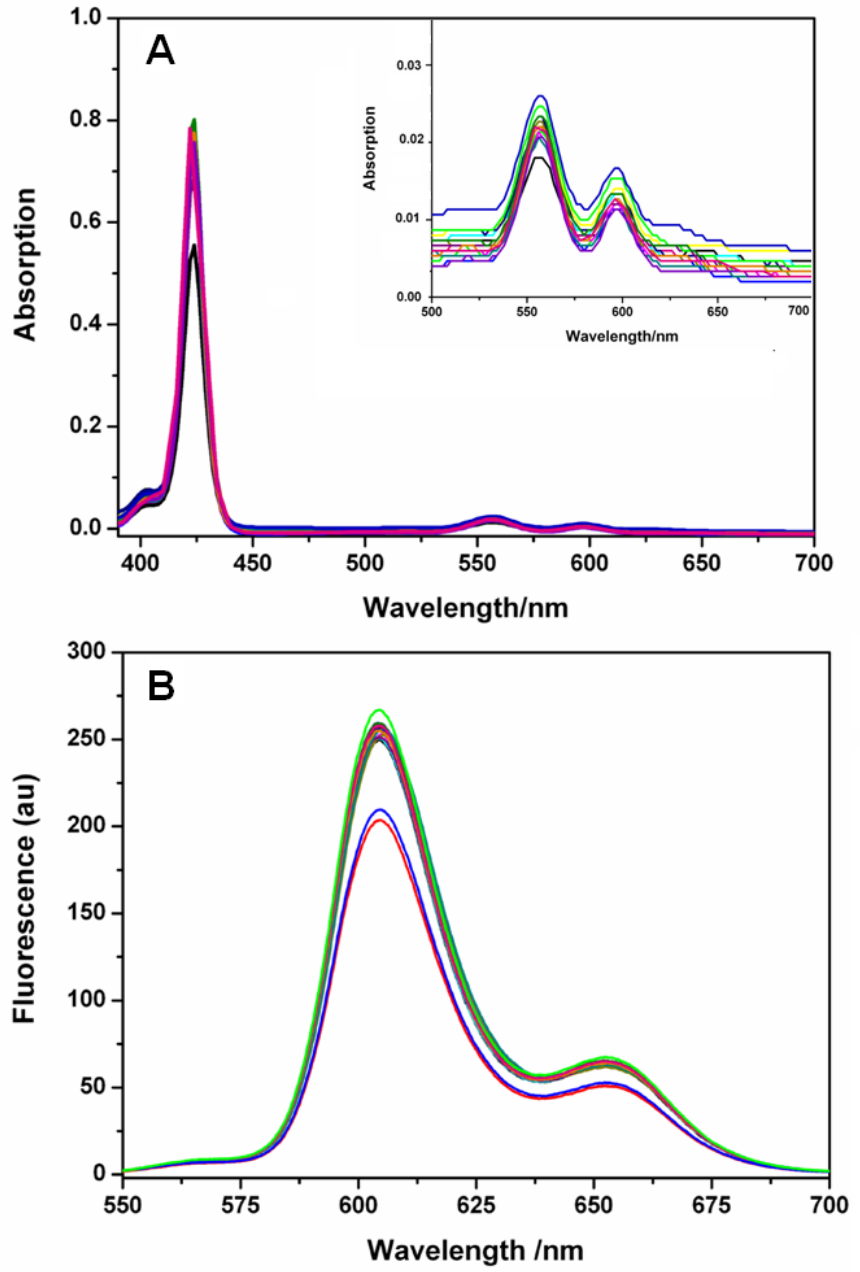

Figure S16. The electronic absorption (A) and fluorescence emission spectra (B) of **1Zn** (2 μM) in CH_2Cl_2/MeOH (1:1) upon addition of Pb^{2+}, Cu^{2+}, Fe^{2+}, Co^{2+}, Hg^{2+}, Mn^{2+}, Zn^{2+}, Ni^{2+}, Cd^{2+}, Ca^{2+}, Ba^{2+}, Mg^{2+}, Li^{+}, Na^{+}, or K^{+} (10 equiv), respectively, with the excitation of 420 nm.

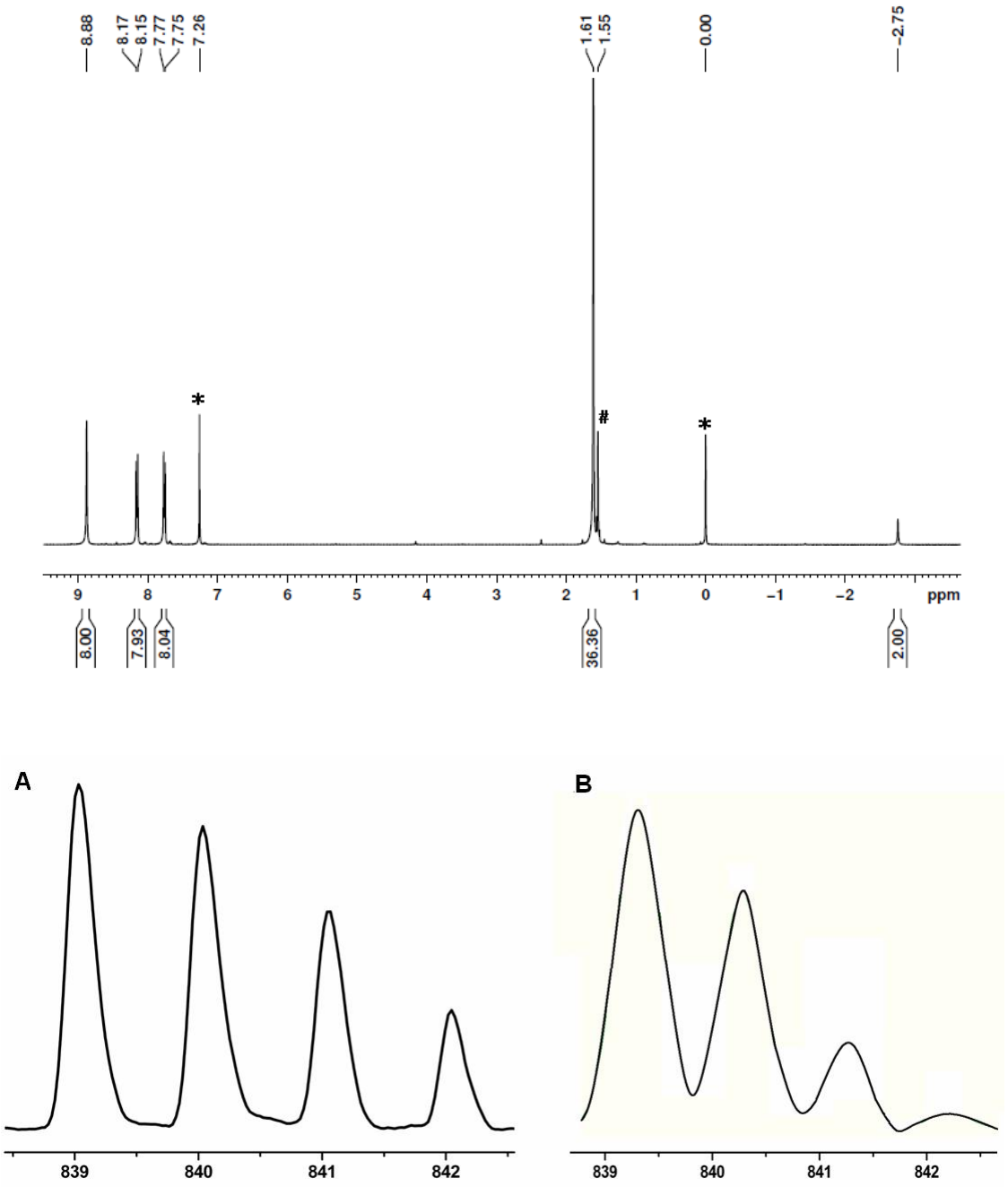

Figure S17. ^{1}H NMR spectrum (Top) of metal free 5,10,15,20-tetra (4-tert-butylphenyl) porphyrin in $CDCl_3$; experimental and simulated isotopic pattern (bottom A and B) for its molecular ion shown in the MALDI-TOF mass spectrum. *and # indicate the residual solvent signals of $CHCl_3$ and H_2O impurities, respectively.

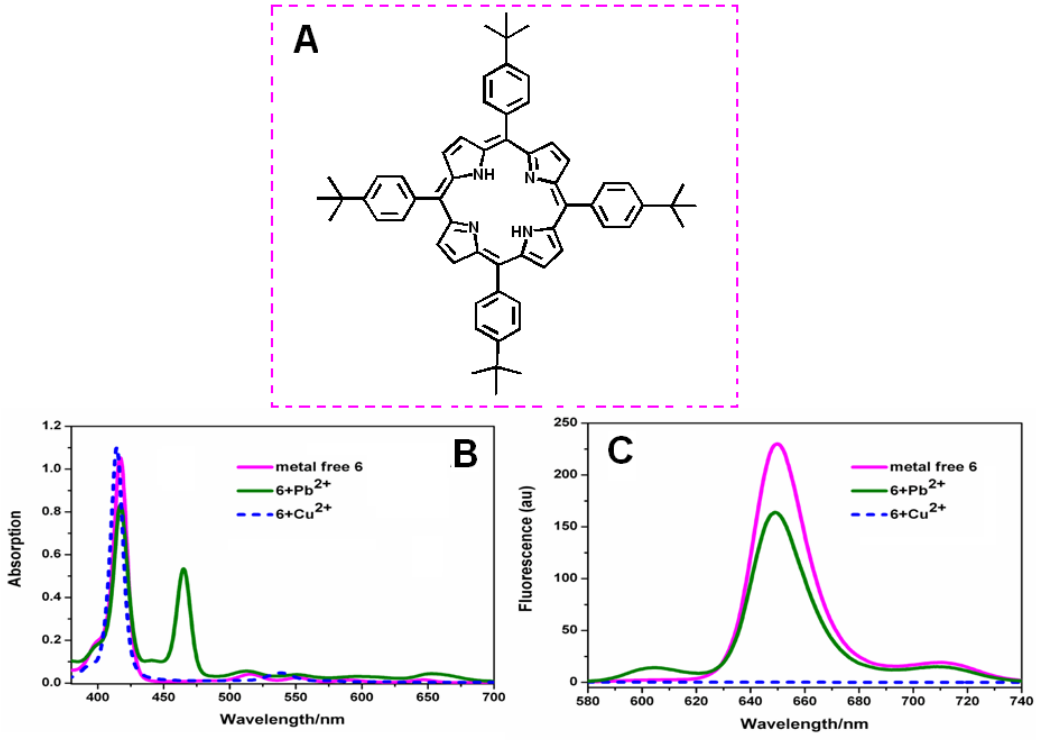

Figure S18. The schematic molecular structure (A) of metal free 5,10,15,20-tetra(4-tert-butylphenyl)porphyrin together with its electronic absorption (B) and fluorescence emission spectra (C) (2 μM) in CH_2Cl_2/MeOH (1:1) upon addition of Pb^{2+} and Cu^{2+} (10 equiv), respectively, with the excitation of 420 nm.