

Electronic Supplementary Information

AIE Active Fluorescent Organic Nanoparticles based Optical Detection of Cu²⁺ ion in Pure Water: A Case of Aggregation-disaggregation Reversibility

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General methods for characterization

¹H-NMR and ¹³C-NMR spectra were recorded with a Bruker Advance DRX 400 spectrometer (Billerica, Massachusetts, USA) operating at 400 and 100 MHz respectively. Chemical Shifts are reported in ppm downfield from the internal standard: TMS, for ¹H-NMR. FTIR spectra were recorded on a Perkin-Elmer FT-IR Spectrum BX system (PerkinElmer, Massachusetts, USA). Mass spectra were recorded on Micro mass Q-TOF Micro TM spectrometer (Bruker, Massachusetts, USA). Elemental analysis was recorded using Thermo Finnigan EA FLASH 1112 SERIES (Thermo Finnigan, California, United States).

Synthesis of 1: The synthesis of **1** has been performed following the procedure reported in the literature. 1-pyrenyl aldehyde (0.64 g, 2.8 mmol), 2-acetyl pyridine (0.67 g, 5.5 mmol), acetamide (3.94 g, 67 mmol) and ammonium acetate (3 g, 37.7 mmol) were taken in a round bottom flask and heated at 180°C for 3 h with stirring. Subsequently, NaOH solution (10 % v/v: NaOH in excess) was added to the reaction mixture and heated at 120°C for a further 2 h without stirring. The reaction mixture was then extracted with CHCl₃ and the crude product was purified over silica gel chromatography using hexane-ethyl acetate as mobile phase (while powder, yield: 62 %).

Characterization: ¹H-NMR (500 MHz, CDCl₃): δ 7.35-7.39 (m, 2H), 7.9-7.94 (m, 2H), 8.02-8.28 (m, 9H), 8.68-8.7 (m, 2H), 8.74-8.78 (m, 4H), ¹³C NMR (100 MHz, CDCl₃): δ 155.8, 154.3, 151.8, 148.6, 137.3, 135.0, 132.1, 131.4, 130.5, 128.7, 128.3, 128.0, 127.8, 127.2, 126.5, 125.7, 125.2, 124.9, 124.5, 124.3, 124.0, 123.2, 122.5. EI MS: m/z 433 (M⁺). Anal calcd. for C₃₁H₁₉N₃: calcd: C 85.89 %, H 4.42 %, N 9.69 %; found: C 86.08 %, H 4.54 %, N 9.68 %.

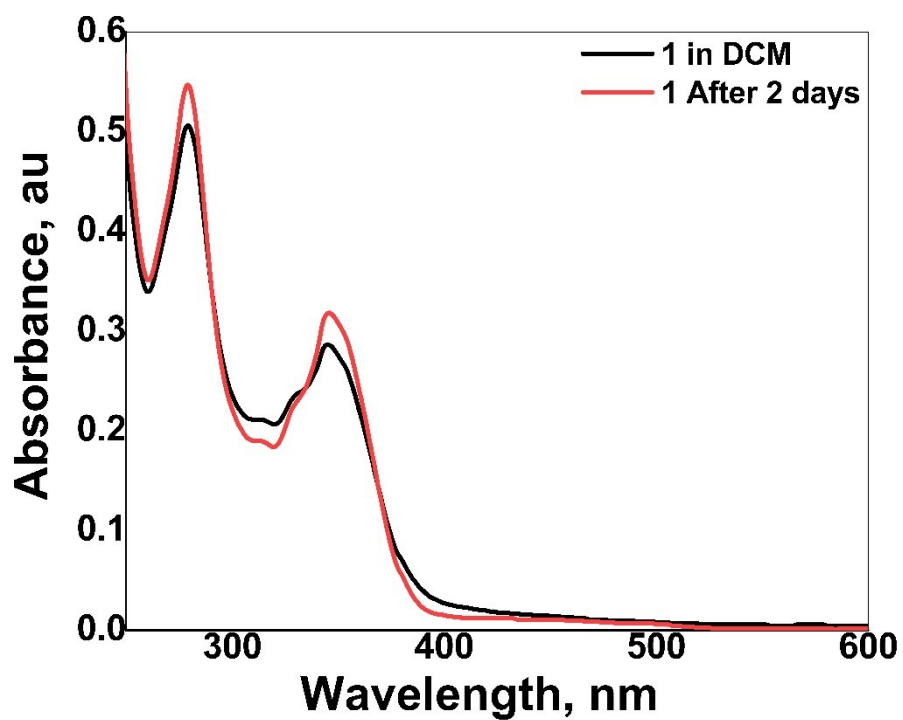


Figure S1: Absorption spectra of 1 (10 μ M) in DCM with a gap of 2 days.

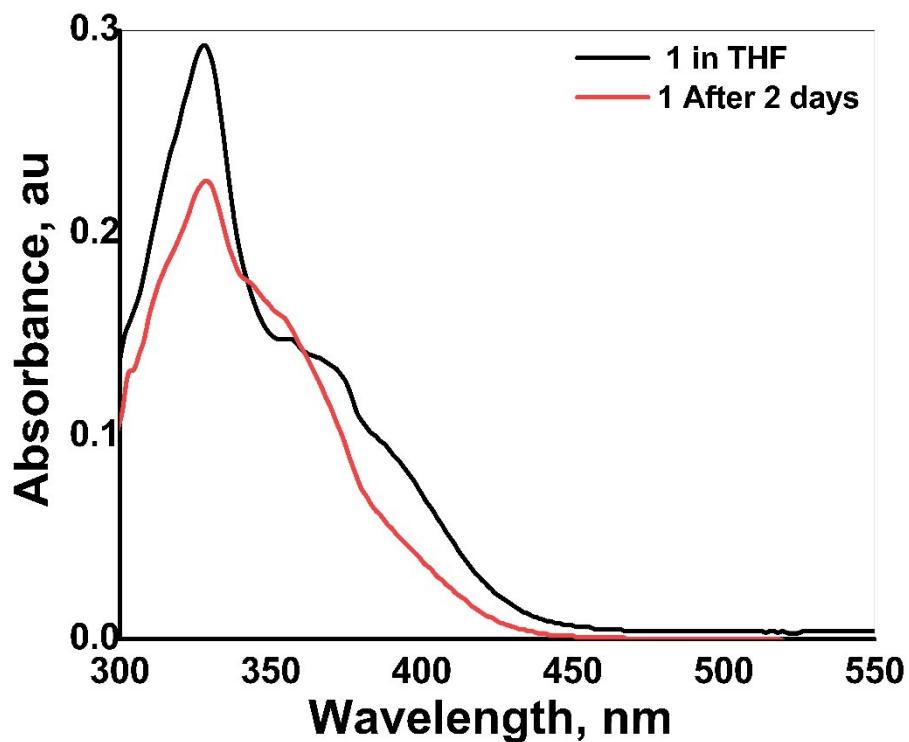


Figure S2: Absorption spectra of 1 (10 μ M) in THF with a gap of 2 days.

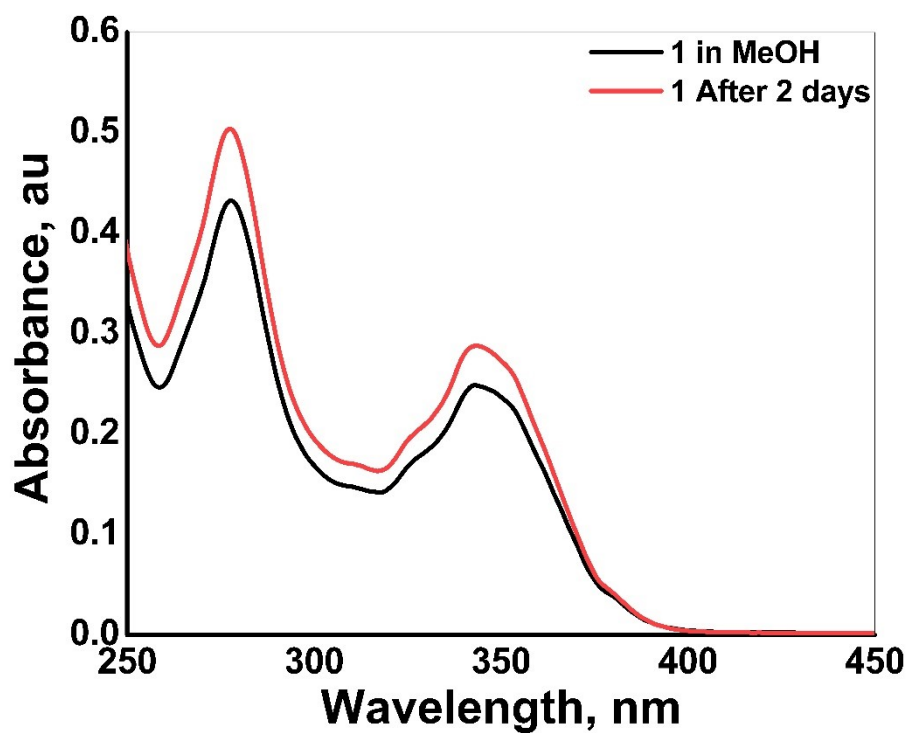


Figure S3: Absorption spectra of 1 (10 μ M) in MeOH with a gap of 2 days.

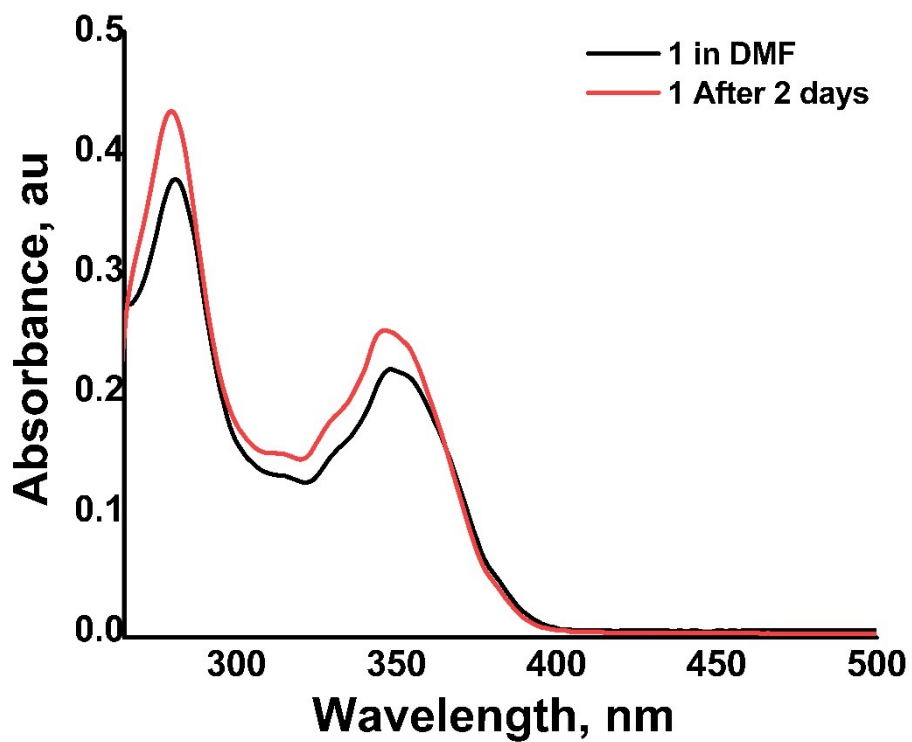


Figure S4: Absorption spectra of 1 (10 μ M) in DMF with a gap of 2 days.

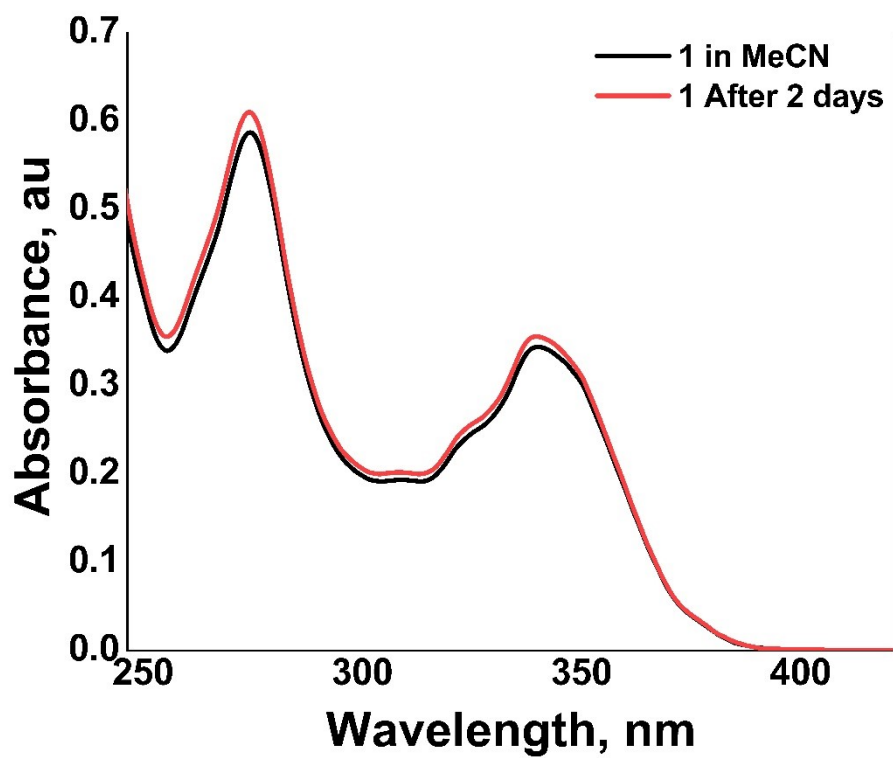


Figure S5: Absorption spectra of **1** (10 μ M) in MeCN with a gap of 2 days.

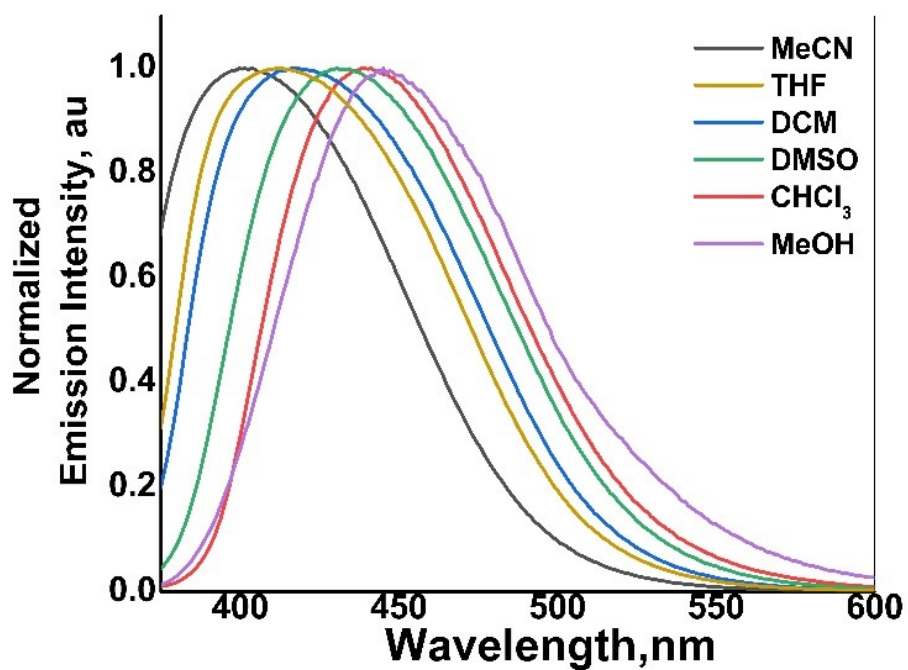


Figure S6: Normalised emission spectra of **1** (10 μ M) in different solvents (λ_{ex} = 340 nm).

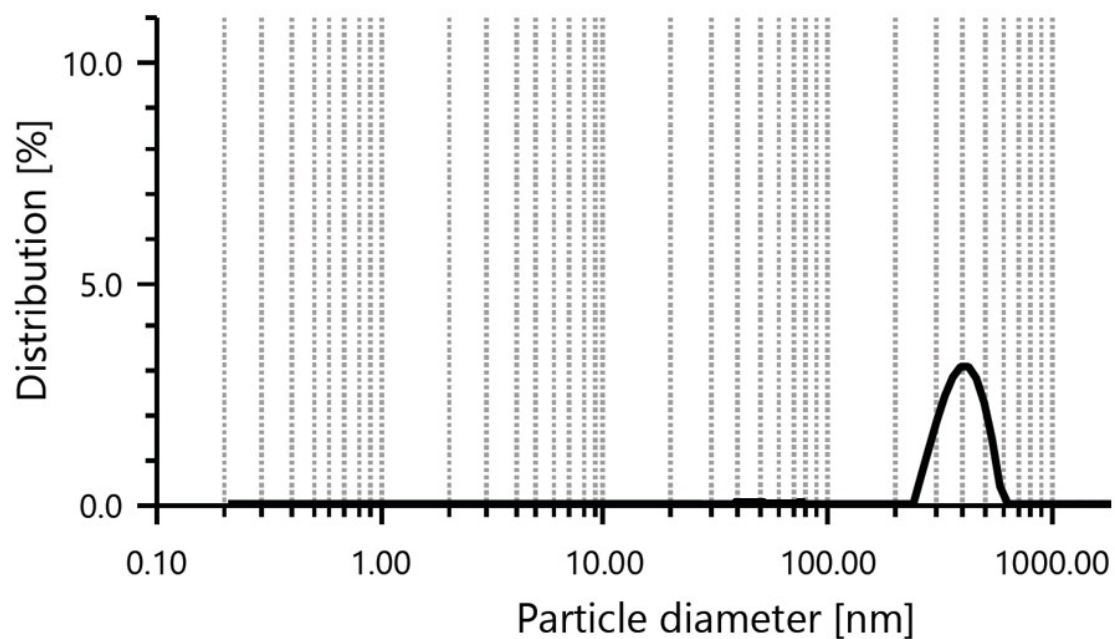


Figure S7: DLS size distribution plot of suspension 1 in water.

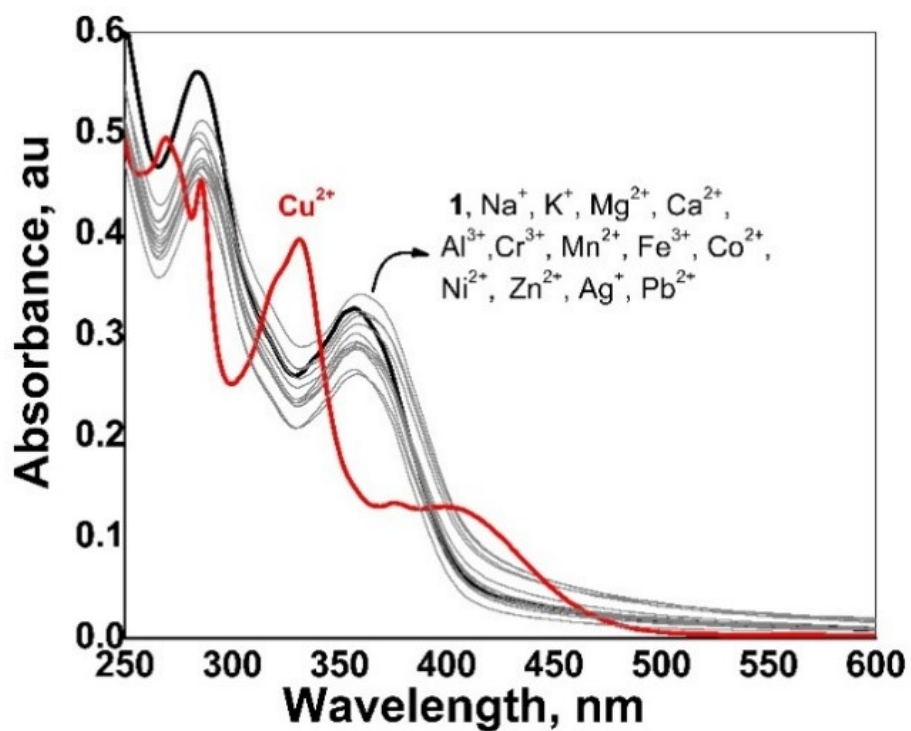


Figure S8: Absorption spectral selectivity of 1 (10 μM) in the presence of different metal ion salts (300 μM) in water.

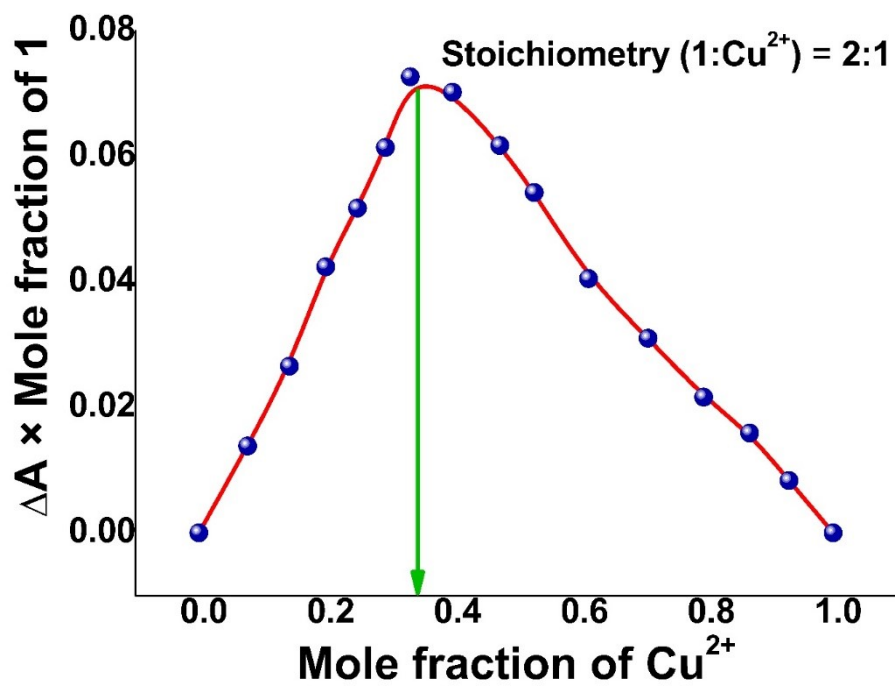


Figure S9: Job's plot of **1** ($10 \mu\text{M}$) with different mole fraction of CuCl_2 in water.

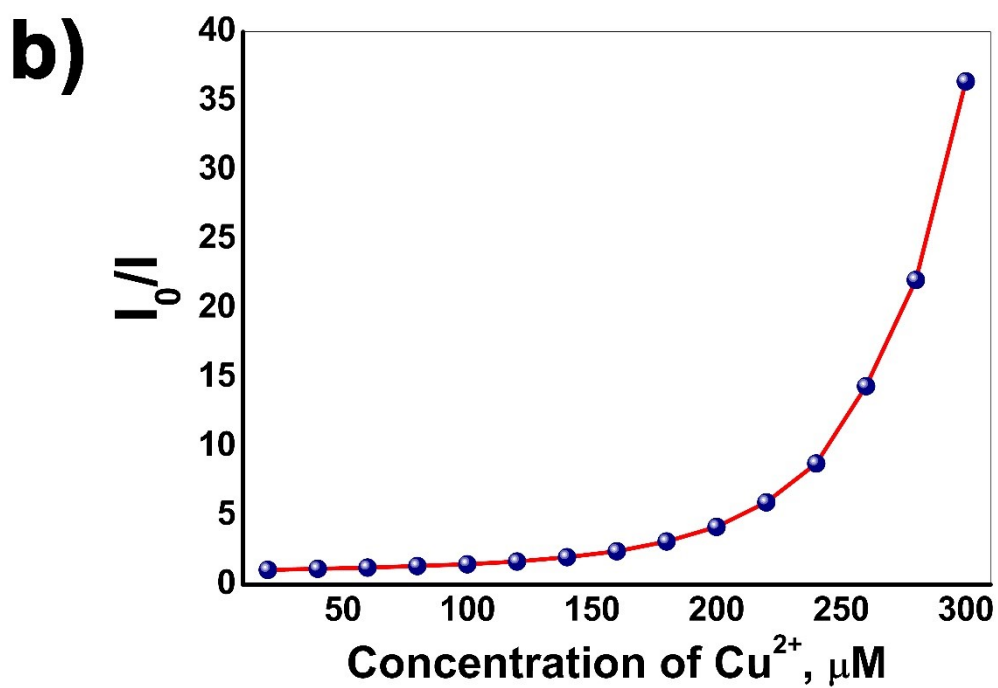
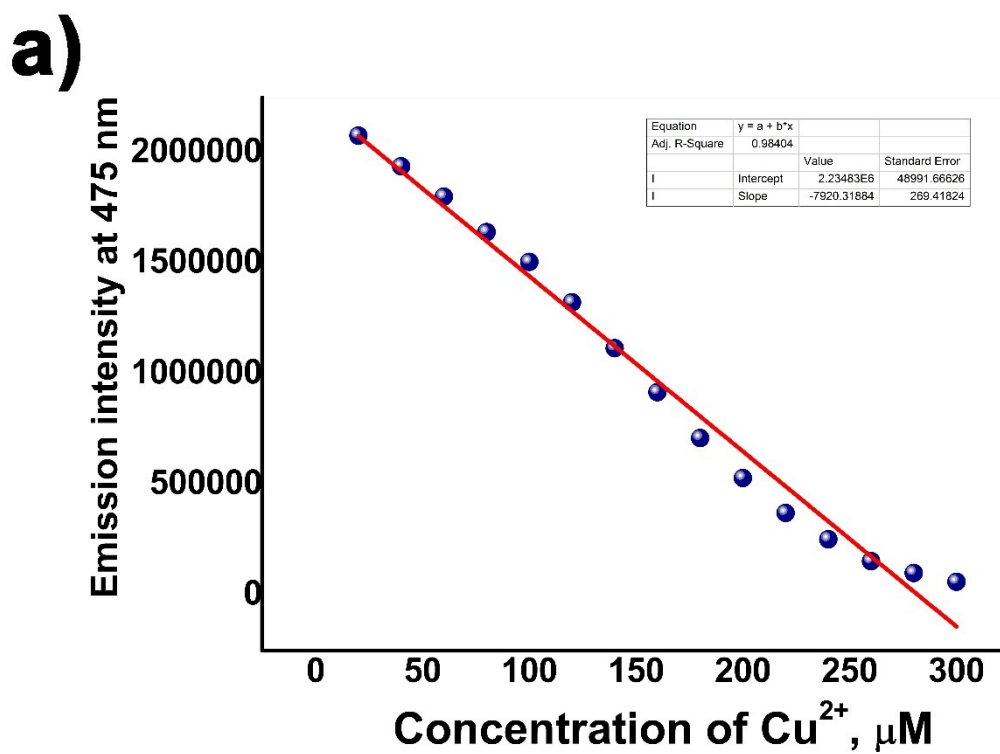


Figure S10: a) Linear fit curve of the fluorescence titration of **1** with CuCl_2 ; b) SV plot. ($[\mathbf{1}] = 10 \mu\text{M}$; $[\text{Cu}^{2+}] = 0\text{-}300 \mu\text{M}$; $\lambda_{\text{ex}} = 340 \text{ nm}$, $\lambda_{\text{em}} = 475 \text{ nm}$) in water.

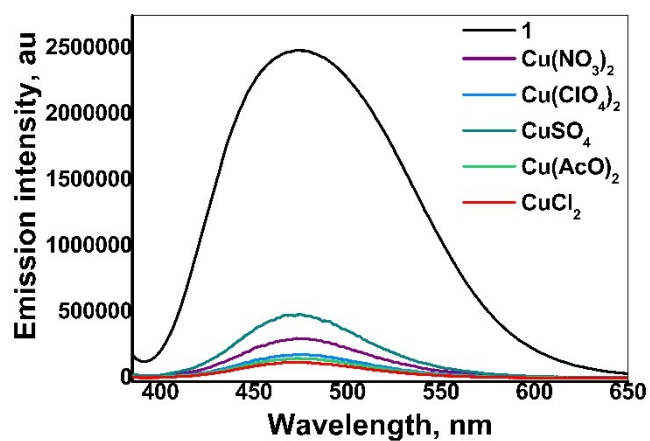


Figure S11: Emission spectral change of **1** (10 μM) in presence of different Cu^{2+} ion salts (300 μM) in water ($\lambda_{\text{ex}} = 340 \text{ nm}$).

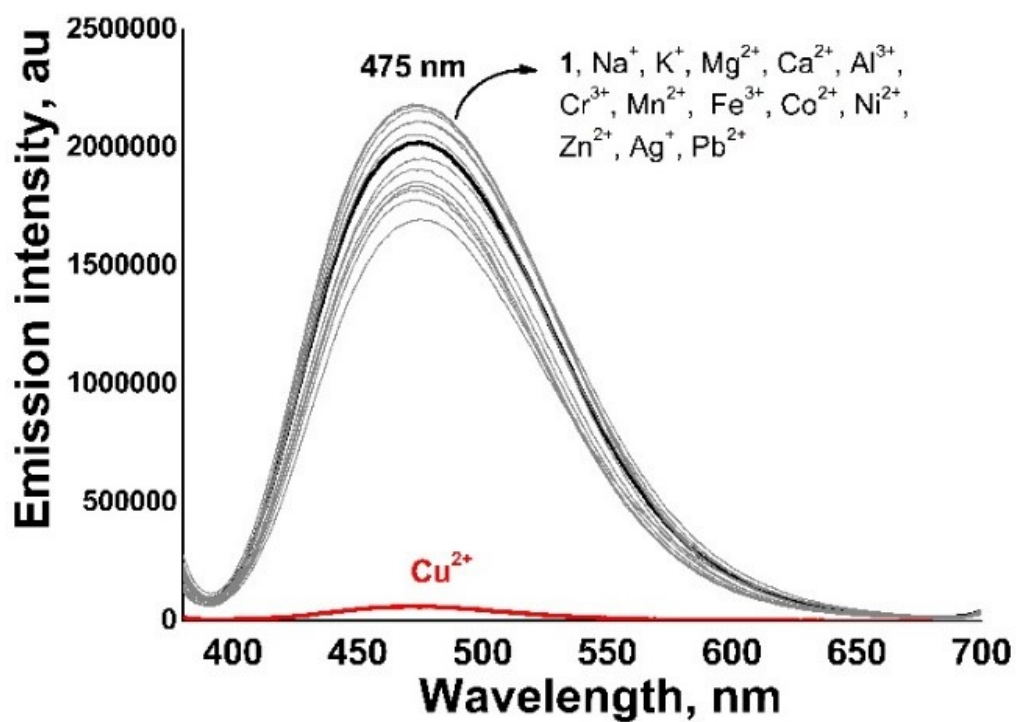


Figure S12: Emission spectral selectivity of **1** (10 μM) in the presence of different metal ion salts (300 μM) in water ($\lambda_{\text{ex}} = 340 \text{ nm}$).

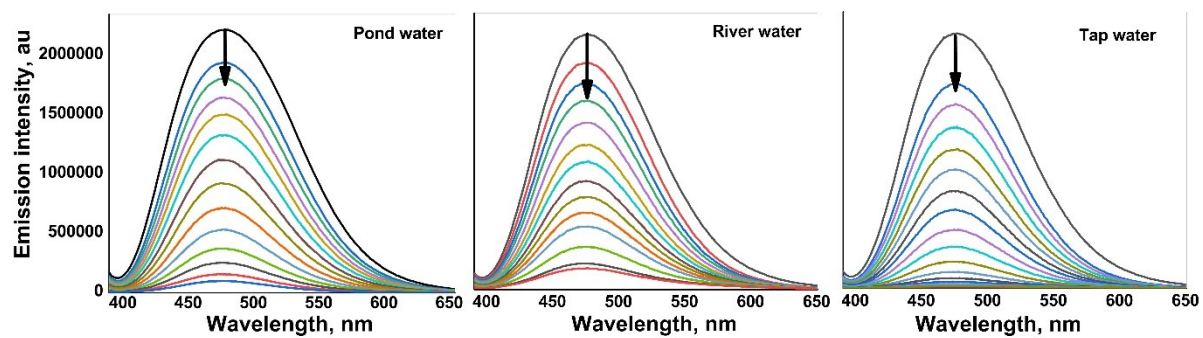


Figure S13: Emission spectral titration of **1** (10 μM) with the gradual addition of CuCl₂ (0-300 μM) in pond water, river water and tap water ($\lambda_{\text{ex}}=340$ nm).