Supporting Information

A turn-on fluorescence BOPHY probe for Cu²⁺ ions

detection

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Figure S1. ¹H-NMR (500 MHz) spectrum of BOPHY-PTZ in CDCl₃.



Figure S2. ¹³C-NMR (125 MHz) spectrum of BOPHY-PTZ in CDCl₃.



Figure S3. IR spectrum of BOPHY-PTZ.



Figure S4. MS spectrum of BOPHY-PTZ.



Figure S5. UV-vis absorption (a) and fluorescence emission (b) spectra of compound 2, compound 3, and BOPHY-PTZ in acetonitrile (2 μ M).

Compound	Absorption (nm)	$\Phi_{\rm F}$
2	258, 312, 438, 458	0.95ª
3	251, 307	0.01 ^b
BOPHY-PTZ	256, 310, 530	0.002°

Table S1. Photophysical data of compounds in acetonitrile.

Fluorescence quantum yield was obtained using a reference method. ^aDiphenylanthracene ($\Phi = 0.85$ in benzene) was used as a standard (excited at 390 nm). ^bQuinine sulfate ($\Phi = 0.52$ in 0.05 M H₂SO₄) was used as standard (excitation at 350 nm). ^cRhodamine 6G ($\Phi = 0.95$ in EtOH) was used as the standard (excitation at 530 nm).



Figure S6. MS spectrum of BOPHY-PTZO. Sample solution was prepared by mixing BOPHY-PTZ (2 μ M) with Cu²⁺ (20 μ M) in CH₃CN-H₂O solvent mixture (CH₃CN: 99.75%) for 10 min at an ambient temperature.



Figure S7. Cyclic voltammogram of BOPHY-PTZ, scan rate: 50 mV·s⁻¹. (Left): in CH₃CN, (right): in H₂O.

Compound	E _(ox) [V] vs NHE	E ₀₋₀ eV ^c	E _{LUMO} (eV) ^d	E _{HOMO} (eV) ^d	E _g (eV) ^e	E _{HOMO} (eV) ^f	E _{LUMO} (eV) ^g	∆G (eV) ^h
BOPHY-PTZ	0.90 ^a 0.83 ^b	2.15	-2.47	-4.99	2.52	-5.03	-2.88	-0.29 0.68
BOPHY-PTZO			-2.47	-5.19	2.72			

Table S2. Electrochemical data and energy levels of BOPHY-PTZ and BOPHY-PTZO.

^aE_(ox) = E_{(ox)-Ag/AgCl} + 0.197, E_{(ox)-Ag/AgCl} is the ground state oxidation potential (first oxidation peak) of the BOPHY-PTZ which is measured with Ag/AgCl as the reference electrode in acetonitrile. ^bE_(ox) = E_{(ox)-SCE} + 0.242, E_{(ox)-SCE} is the ground state oxidation potential (first oxidation peak) of the BOPHY-PTZ which is measured with SCE as the reference electrode in acetonitrile. ^cE₀₋₀ was determined from the edge of the absorption spectrum. ^dThe HOMO and LUMO energy levels were obtained using density functional theory (DFT) at B3LYP/6-31G*. ^cE_g = E_{LUMO} - E_{HOMO}. ^fE_{HOMO} = -(4.8 - E_{FC} + E_{(ox)-Ag/AgCl}) eV. E_{FC} was redox potential of Fc/Fc⁺ vs Ag/AgCl. ^gE_{LUMO} = E_{HOMO} - E₀₋₀. ^h Δ G = E_{ox} - E_{red} - e²/dε, E_{ox} is the oxidation potential of BOPHY-PTZ and E_{red} is the reduction potential of Cu²⁺ in acetonitrile or water, d is the center to center distance of the donor and acceptor and ϵ is the dielectric constant of the solvent. In acetonitrile or water, the coulombic term can be neglected.



Figure S8. Fluorescence emission spectra of 1 μ M BOPHY-PTZ in the absence or presence of 10 μ M Cu²⁺ in different solvents.



Figure S9. Fluorescence emission intensity changes of 1 μ M BOPHY-PTZ at 574 nm in the presence of 10 μ M Cu²⁺ ions in different pH buffer-CH₃CN (CH₃CN: 99.75%) solvent mixtures.



Figure S10. Fluorescence emission intensity changes of 1 μ M BOPHY-PTZ at 574 nm in the absence or presence of 10 μ M Cu²⁺ in different CH₃CN-H₂O solvent mixtures [CH₃CN (v/v %): 99.75, 89.75, 79.75, 49.75 and 19.75%].



Figure S11. Temperature-dependent fluorescence emission intensity changes of BOPHY-PTZ (1 μ M) at 574 nm in CH₃CN-H₂O solvent mixtures (CH₃CN: 99.75%) in the presence or absence of Cu²⁺ (10 μ M).



Figure S12. Time-dependent fluorescence emission intensity changes of BOPHY-PTZ (1 μ M) at 574 nm in CH₃CN-H₂O solvent mixture (CH₃CN: 99.75%) and in the presence of different concentrations of Cu²⁺ at 20 °C.



Figure S13. (a) Fluorescence spectra of **BOPHY-PTZ** (1 μ M) upon the addition of oxidants and Cu⁺. (b) Fluorescence emission intensity changes of **BOPHY-PTZ** (1 μ M) at 574 nm in the presence of Cu²⁺ (2 μ M) and other anions (20 μ M each). (1) Cu²⁺, (2) O_{2⁻}, (3) MnO_{4⁻}, (4) Cr₂O_{7⁻}, (5) NO_{2⁻}, (6) NO, (7) ClO⁻, (8) Cu⁺.