Synthesis, crystal structure and living cell imaging of a Cu\textsuperscript{2+}–specific molecular probe

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**Figure S1.** Job plot for determining the stoichiometry of 4 and Cu$^{2+}$. The total concentration of 4 and copper was 10×10$^{-5}$ M. $A_0$ and $A$ are the absorbance values of 4 in the absence of Cu$^{2+}$ and 4 upon addition of different amounts of Cu$^{2+}$.

**Figure S2.** Absorption spectra of 4 with 1 equiv. Cu$^{2+}$ in CH$_3$CN/HEPES (20 mM, pH 7.2, 3:7, v/v) solution. Inset shows the absorbance at 554 nm of 4 as a function of Cu$^{2+}$ concentration.
**Figure S3.** Color changes of 10 μM 4 in the presence of different concentrations of Hg\(^{2+}\) (top) or Cu\(^{2+}\) (bottom), from left to right: 0.1, 0.3, 0.5, 0.7, 1, 2, 3, 10, 30, 50 equiv.

**Figure S4.** The effect of pH (6.9 – 7.5) on the relative fluorescence intensity probe 4 with 30 equiv. Cu\(^{2+}\) in CH\(_3\)CN/HEPES (20 mM, 3:7, v/v) solution. (Excitation wavelength (\(\lambda_{ex}\)), 554 nm; slit width, 10 nm; emission wavelength (\(\lambda_{em}\)), 580 nm; slit width, 4.5 nm.)
Figure S5. FT–IR spectrum of compound 4

Figure S6. $^1$H NMR (CDCl$_3$, 400 MHz) spectrum of compound 4
Figure S7. $^{13}$C NMR (CDCl$_3$, 100 MHz) spectrum of compound 4

Figure S8. HRMS spectrum of compound 4