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## NBD-based Fluorescent Chemosensor for the Selective Quantification of Copper and Sulfide in Aqueous Solution and Living Cells

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Fig. S2  $^{13}$ C-NMR of NL (DMSO- $d_6$ )



Fig. S3 High resolution TOF-MS of NL



Fig. S4 Time-dependent fluorescence changes of NL in HEPES aqueous buffer (THF:  $H_2O = 3.7$ ,

20 mM, pH = 7.4). Excitation at 430 nm.



**Fig. S5** Variations of fluorescence intensity at 519 nm of NL (10  $\mu$ M) in aqueous solution with (bottom) and without (up) Cu<sup>2+</sup> (0–20  $\mu$ M) as a function of pH. Excitation at 430 nm.



**Fig. S6** Absorption spectra of **NL** (10  $\mu$ M) in HEPES aqueous buffer (THF: H<sub>2</sub>O = 3:7, 20 mM, pH = 7.4) upon addition of various metal ions (20  $\mu$ M).



**Fig. S7.** The Job's plot of **NL** toward  $Cu^{2+}$ .



Fig. S8 Linear relationship between fluorescence intensity of NL (1  $\mu$ M) at 519 nm versus the concentration of Cu<sup>2+</sup> in HEPES buffer (THF: H<sub>2</sub>O = 3:7, 20 mM, pH = 7.4). Excitation at 430 nm.



**Fig. S9** UV-vis spectra of **NL** (10  $\mu$ M) sequential in the presence of Cu<sup>2+</sup> (20  $\mu$ M) and S<sup>2-</sup> (20  $\mu$ M) in HEPES aqueous buffer (THF: H<sub>2</sub>O = 3:7, 20 mM, pH = 7.4).



Figure S10 ESI-mass spectra of NL-Cu<sup>2+</sup> ensemble



Figure S11 ESI-mass spectra of NL-Cu<sup>2+</sup> ensemble in the presence of  $S^{2-}$ .



Fig. S12 Flow cytometric analysis of MDA-MB-231 cells stained with NL and its fluorescent response to  $Cu^{2+}$  and  $S^{2-}$ . (a) Control group: MDA-MB-231 cells only, (b) cells stained with 10  $\mu$ M NL for 20 min, (c) NL stained cells treated with 20  $\mu$ M  $Cu^{2+}$  for 15 min, (d) then incubated with 40  $\mu$ M  $S^{2-}$  for another 30 min.