

Electronic supplementary information(ESI)

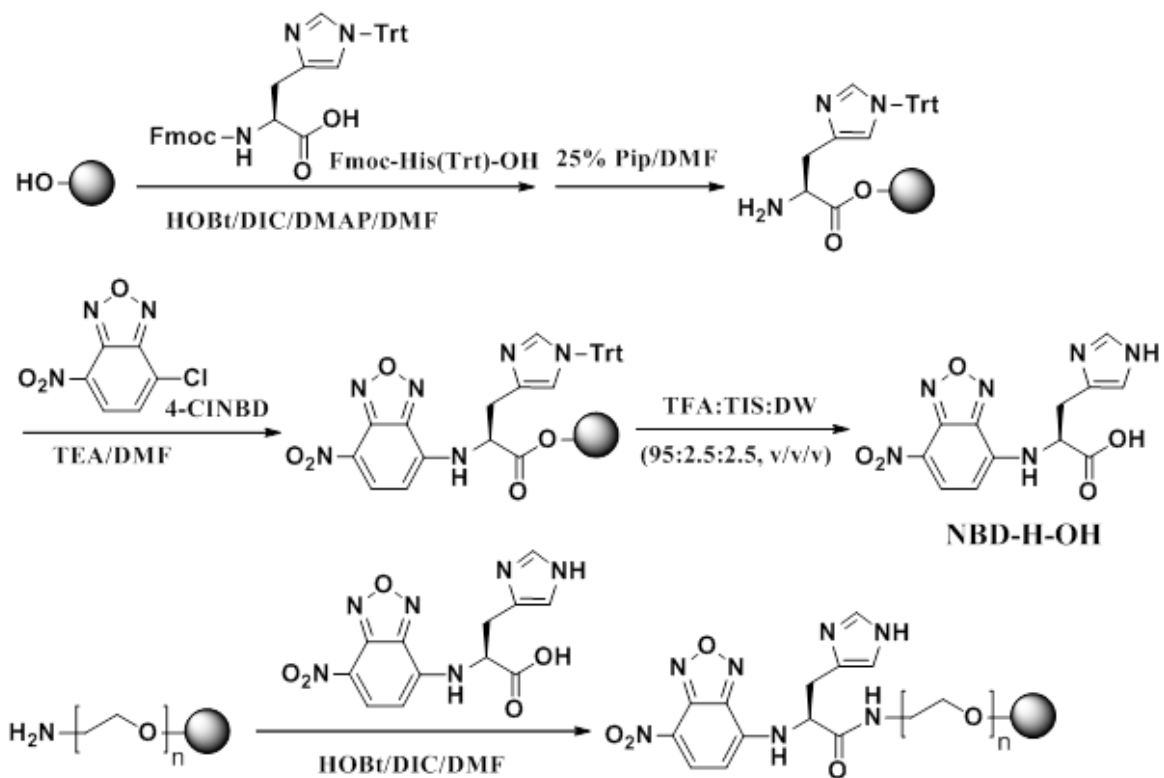
Highly sensitive colorimetric detection and removal of Hg^{II} and Cu^{II} in aqueous solution: From amino acids toward solid platforms

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Scheme S1. Synthesis of NBD-H-PEG-PS

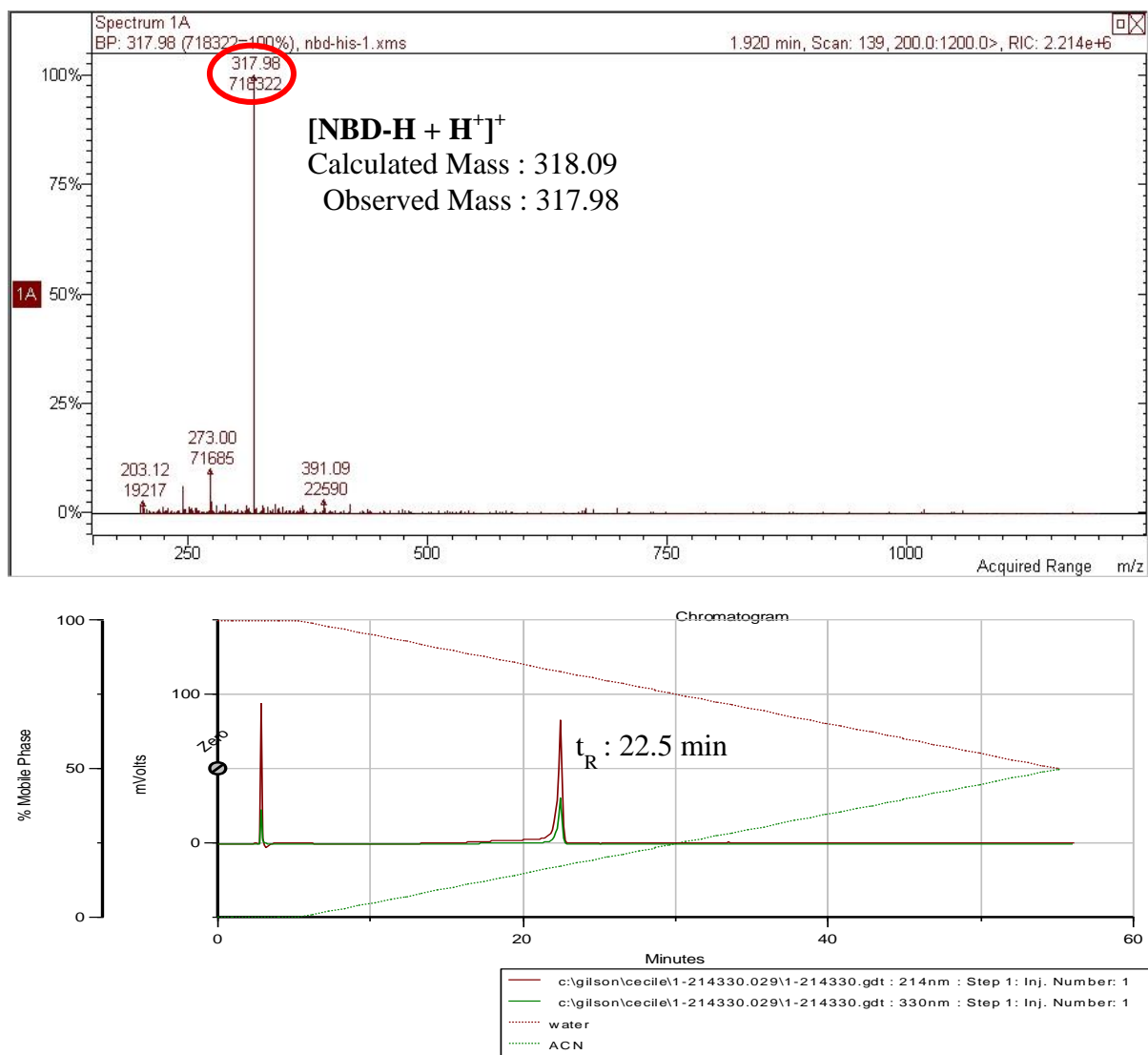


Figure S1. ESI-MS and HPLC spectrum of **NBD-H**

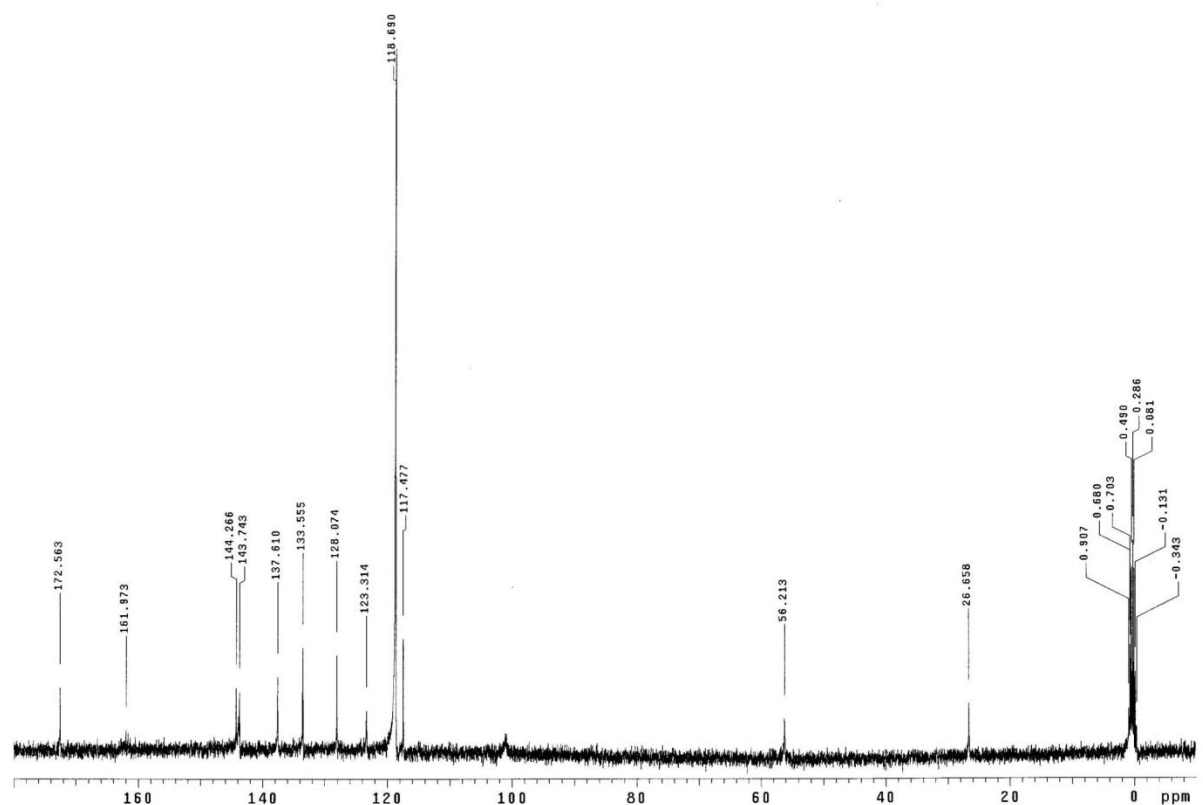
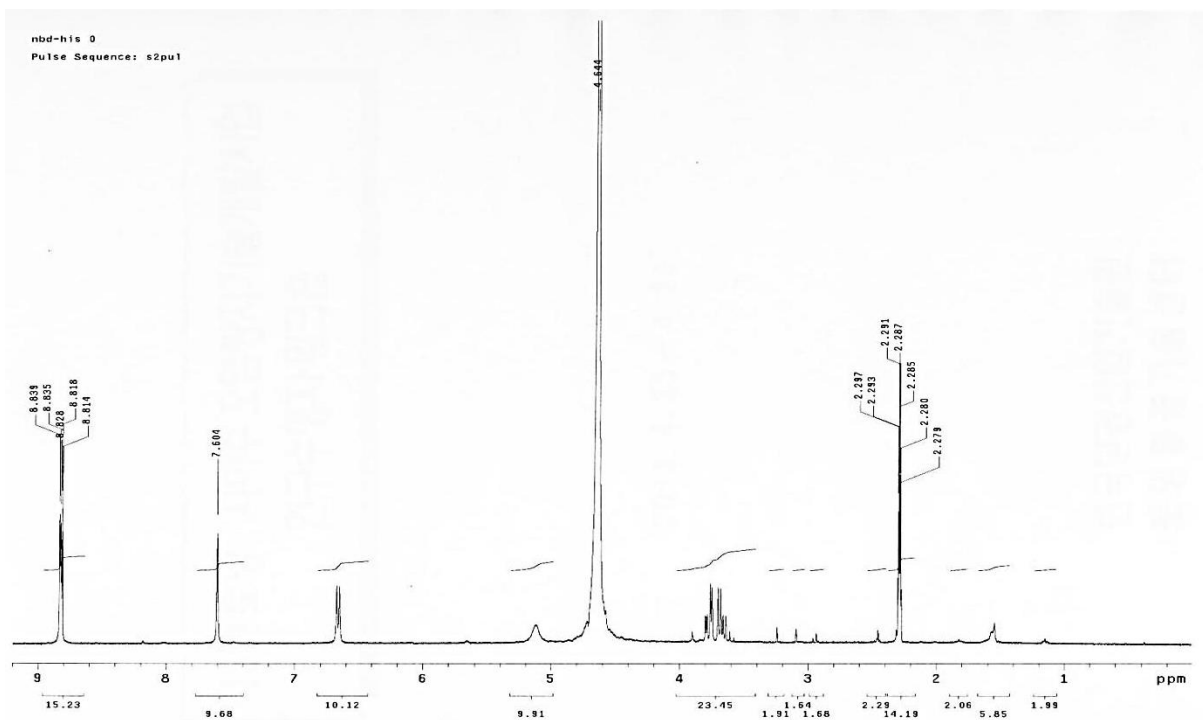


Figure S2. (a) ^1H NMR of NBD-H (15 mM) in 50% ACN- $\text{d}_3/\text{D}_2\text{O}$ and (b) ^{13}C NMR of NBD-H in 50% ACN- $\text{d}_3/\text{D}_2\text{O}$ at 25 °C.

4) NBD-HIS with GLY (POS)

BG_140414_NBD-His_003-c1 #77-100 RT: 1.14-1.48 AV: 24 SB: 14 0.33-0.53 NL: 6.68E3
T: +o FAB Full ms [229.50-380.50]

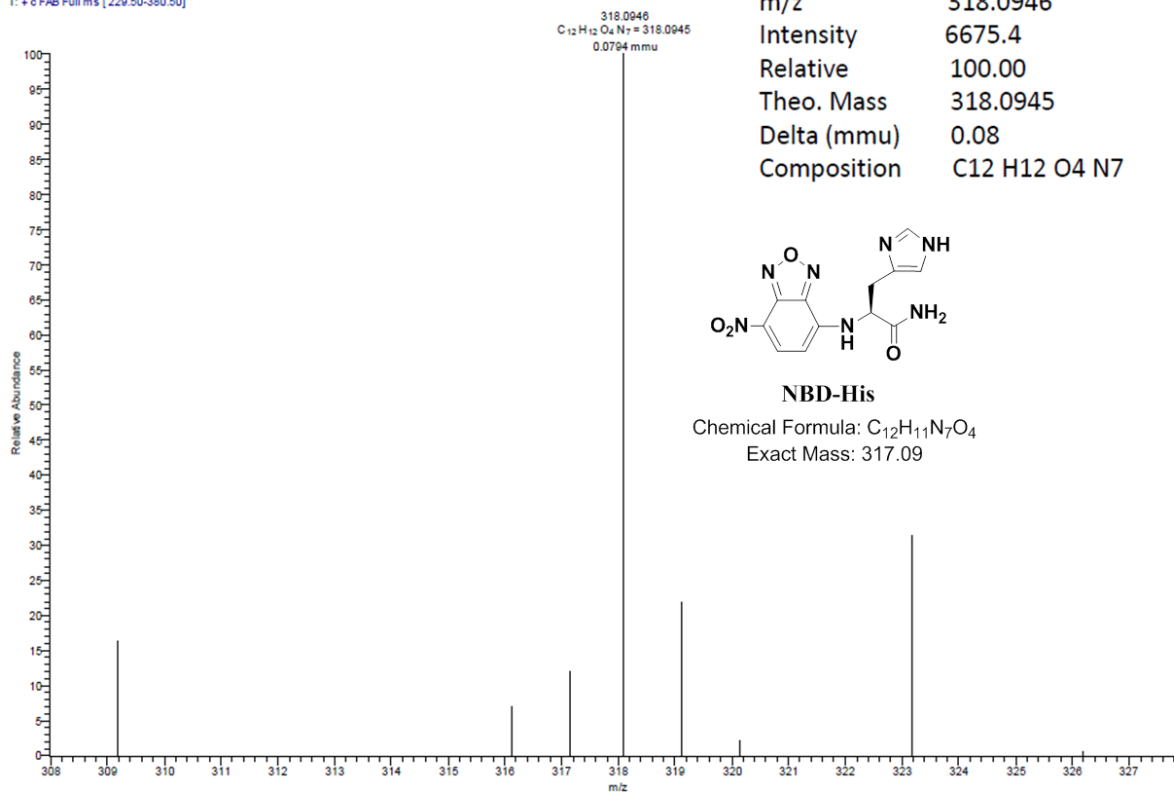


Figure S3. FAB-HRMS spectrum of **NBD-H**

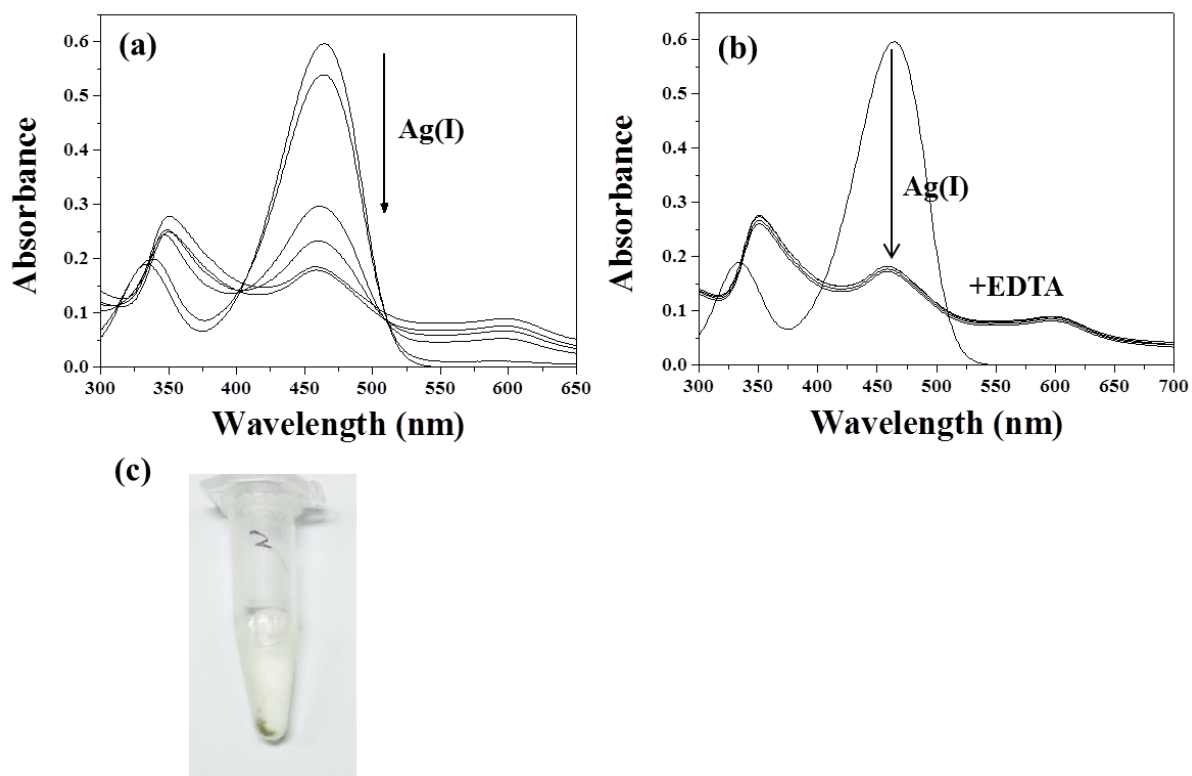


Figure S4. UV-VIS absorbance spectra of **NBD-H** (30 μM) in 10 mM HEPES buffer solution (pH 7.4) containing 3% ACN (a) with increasing concentration of Ag^{I} (0, 20, 40, ..., 100 μM) and (b) EDTA (100, 200, 300 μM) after adding Ag^{I} (100 μM). (d) The centrifuged solution of **NBD-H** with Ag^{I} .

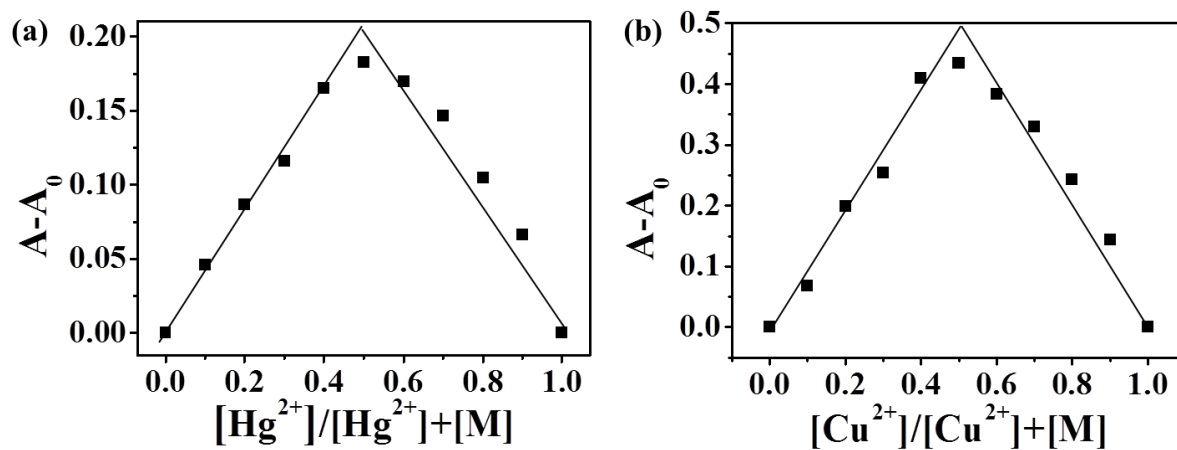


Figure S5. A Job plot for NBD-H (30 μM) with (a) Hg^{II} and (b) Cu^{II} in 10mM HEPES buffer solution (pH 7.4) containing 5% ACN.

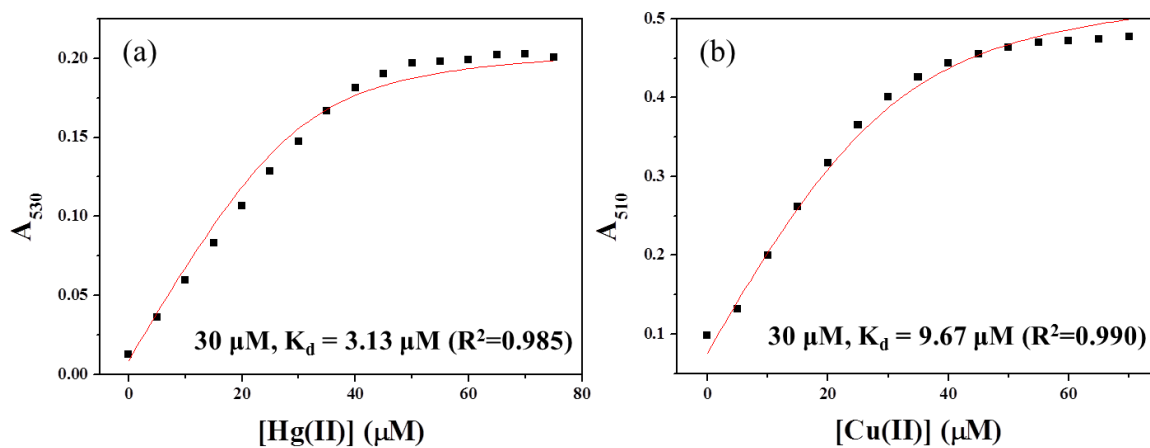
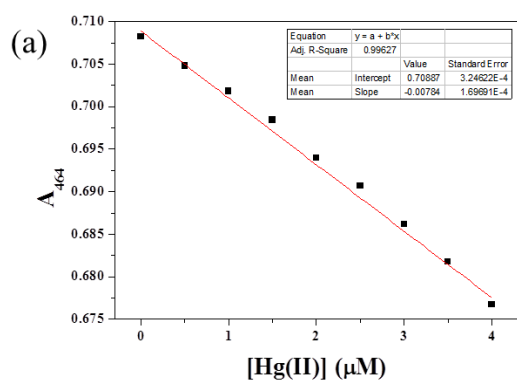
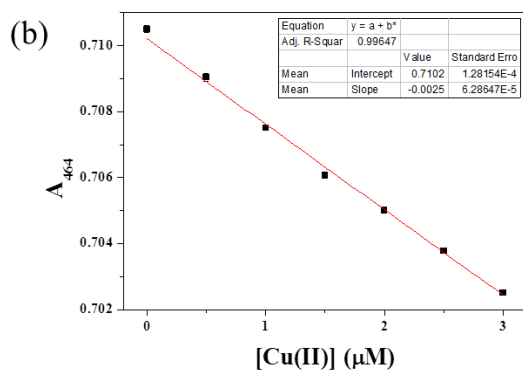


Figure S6. Absorbance titration curve of **NBD-H** (30 μM) in 10 mM HEPES buffer solution (pH 7.4) containing 3% ACN (a) with increasing concentration of Hg^{II} (0, 5, 10, 15, ..., 70, 75 μM) and (b) Cu^{II} (0, 5, 10, 15, ..., 65, 70 μM)



$$\left| \frac{3\sigma}{M} \right| = \left| \frac{3 * 0.00046}{-0.00784} \right| = 0.176 \mu\text{M} \quad (R^2=0.99627)$$



$$\left| \frac{3\sigma}{M} \right| = \left| \frac{3 * 0.000141}{-0.00259} \right| = 0.163 \mu\text{M} \quad (R^2=0.99647)$$

Figure S7. Detection limit of **NBD-H** (30 μM) with (a) Hg^{II} or (b) Cu^{II} ions in 10 mM HEPES buffer solution (pH 7.4) containing 3% ACN.

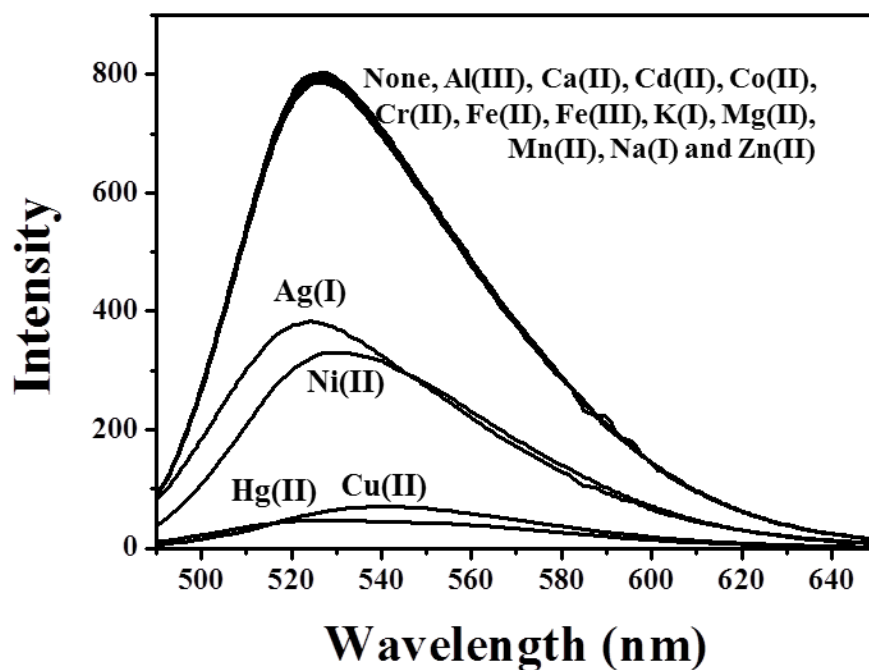


Figure S8. Fluorescence emission spectra of NBD-H (30 μM) in 10 mM HEPES buffer solution (pH 7.4) containing 3% ACN in presence of various metal ions (60 μM).

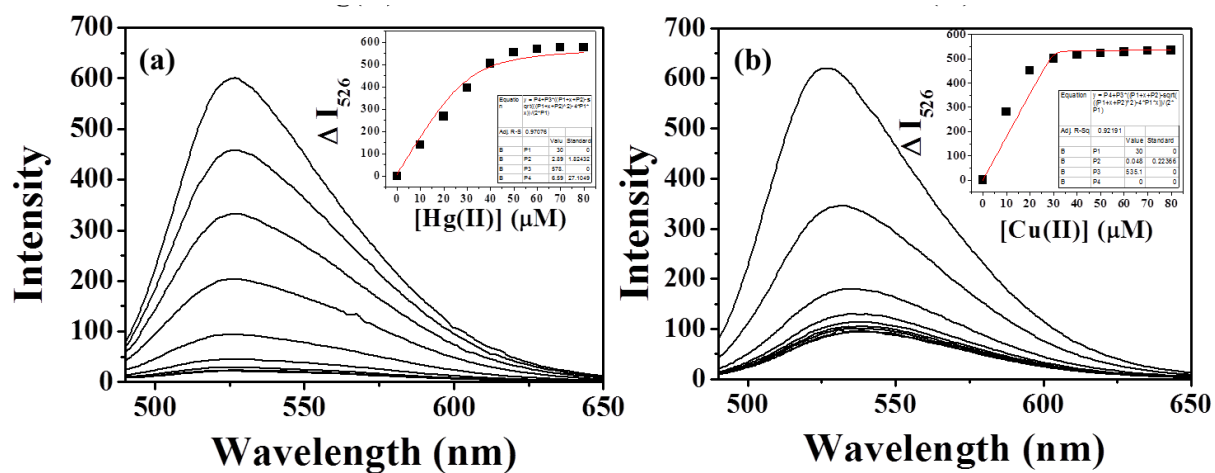


Figure S9. Fluorescence emission spectra of **NBD-H** (30 μM) in 10 mM HEPES buffer solution (pH 7.4) containing 3% ACN (a) with increasing concentration of Hg^{II} and (b) Cu^{II} (0, 10, ..., 80 μM). Inset: Fluorescence titration curve of **NBD-H** (30 μM) with increasing concentration of (a) Hg^{II} and (b) Cu^{II}

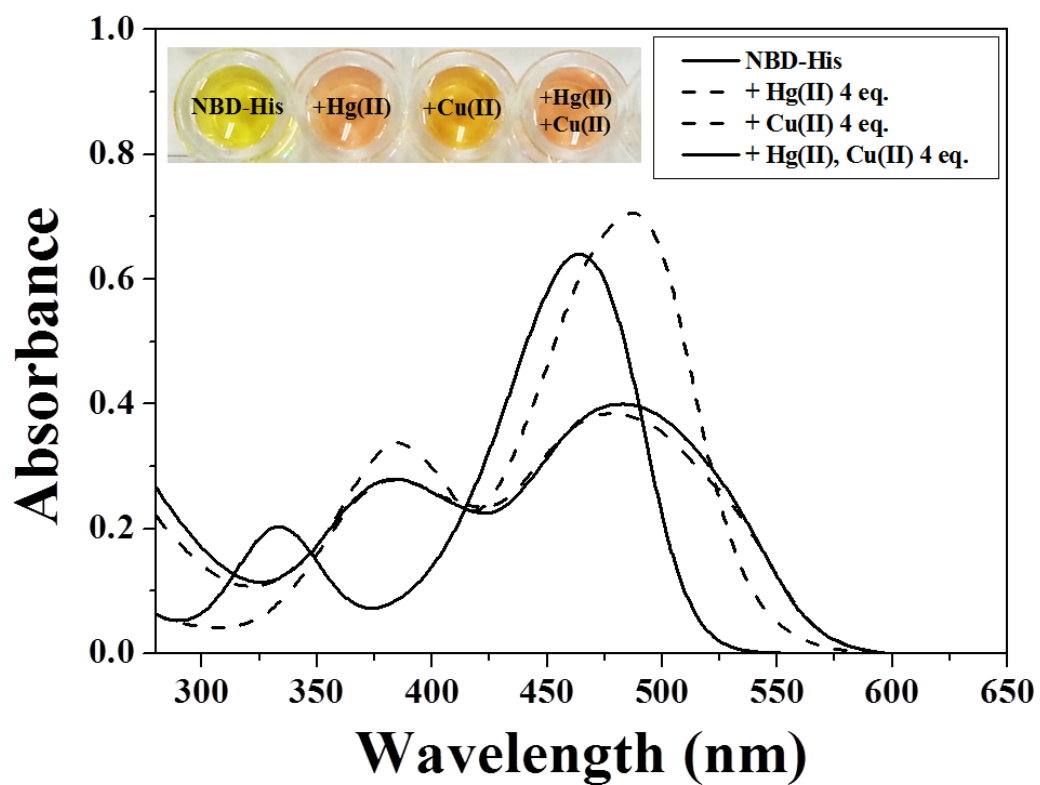


Figure S10. UV-VIS absorbance spectra of NBD-H(30 μM) in 10 mM HEPES buffer solution (pH 7.4) containing 3% ACN in the presence of Hg^{II} and/or Cu^{II}.

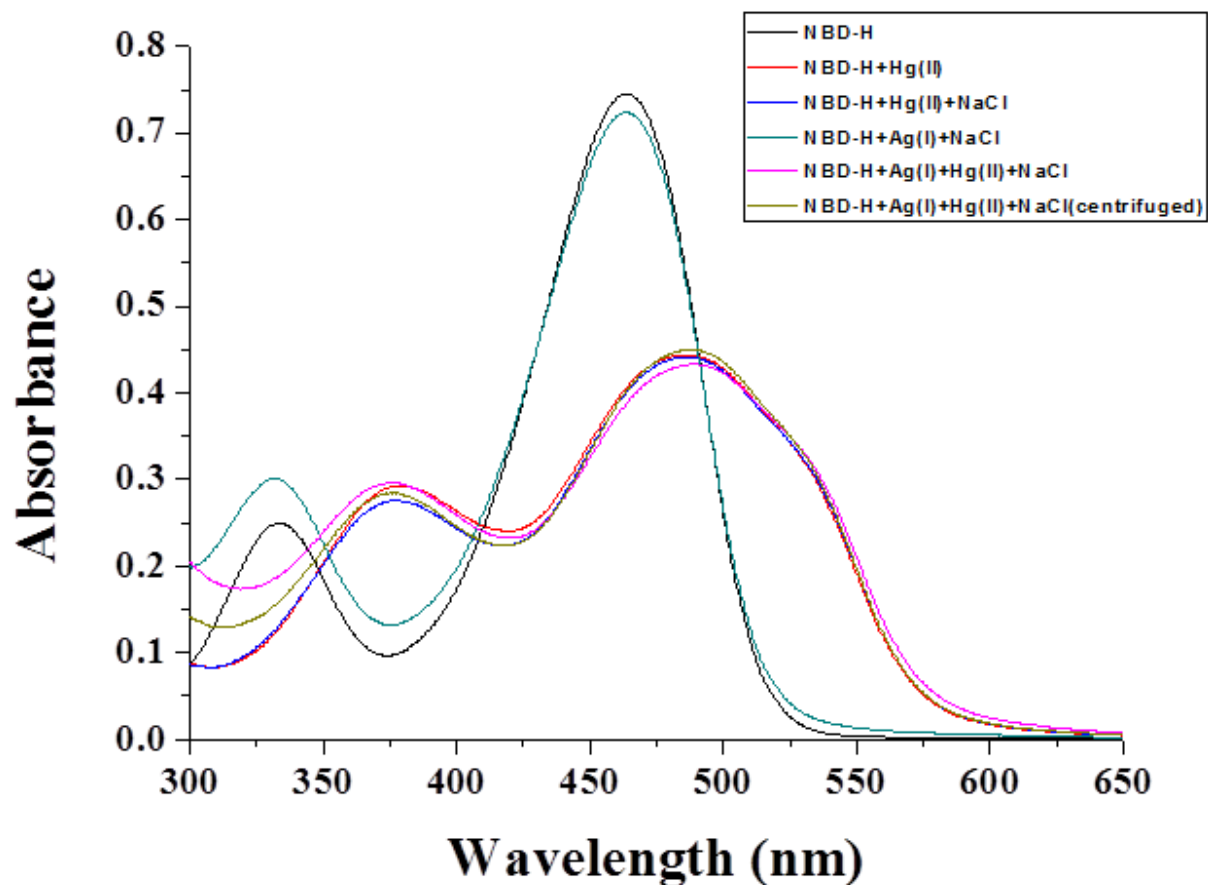


Figure S11. UV-VIS absorbance spectra of **NBD-H** (30 μM) in 10 mM HEPES buffer solution at pH 7.4 containing 3% ACN and 1 mM NaCl in the presence of Ag^{I} (2 equiv.) and/or Hg^{II} (2 equiv.).

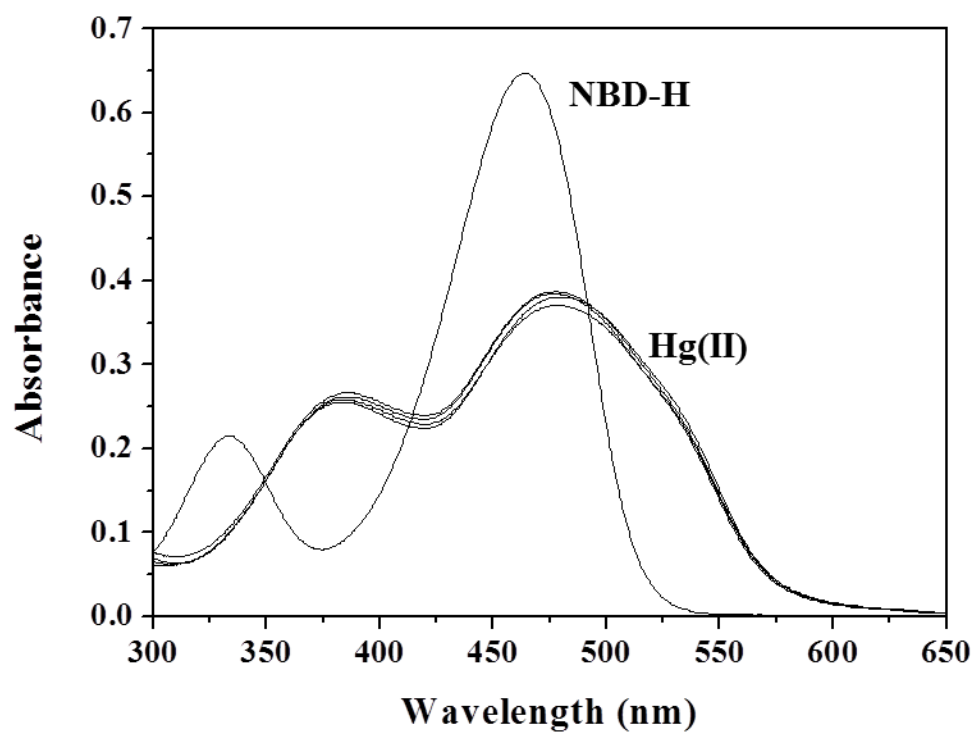


Figure S12. UV-VIS absorbance spectra of **NBD-H** (30 μM) in 10 mM HEPES buffer solution (pH 7.4) containing 3% ACN in presence of 2 equiv. of Hg^{II} (HgCl_2 , $\text{Hg}(\text{OAc})_2$, $\text{Hg}(\text{NO}_3)_2$, and $\text{Hg}(\text{ClO}_4)_2$).

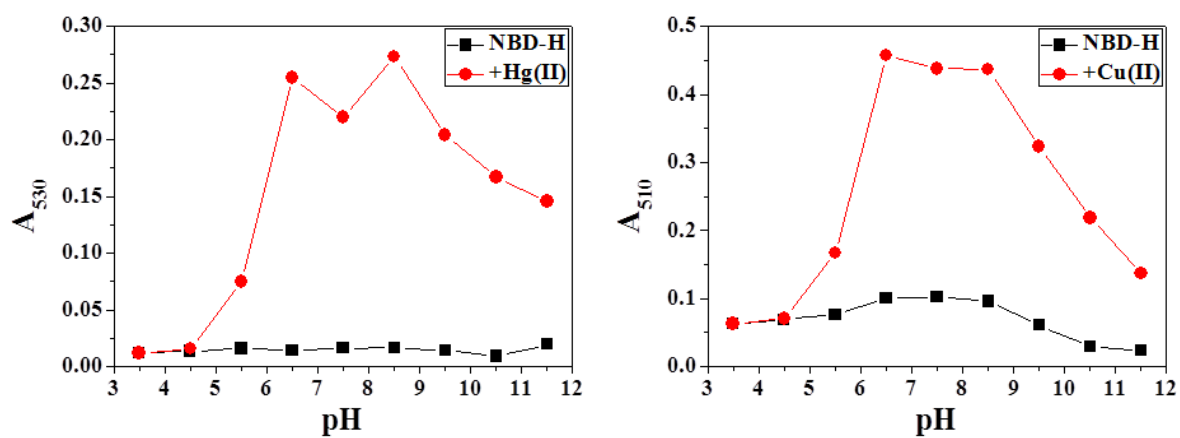


Figure S13. UV/VIS absorbance spectra of **NBD-H** in different pH of 10 mM buffer solution in absence of these metal ions (black line) and in presence of (a) Hg^{II} and (b) Cu^{II} (2 equiv.) (red line)

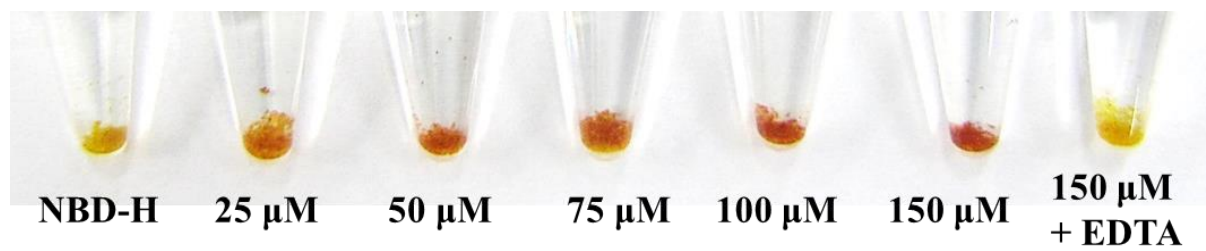


Figure S14. Color change of **NBD-H**-PEG-PS (100 μM) in 10 mM HEPES buffer (pH 7.4) with increasing concentration of Cu^{II} and/or 300 μM EDTA.