Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for

A selective fluorescent probe for the detection of Cd^{2+} in different buffer solutions and water

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Contents:

1. The pH-titration of free NHQ and NHQ/Cd^{2+}

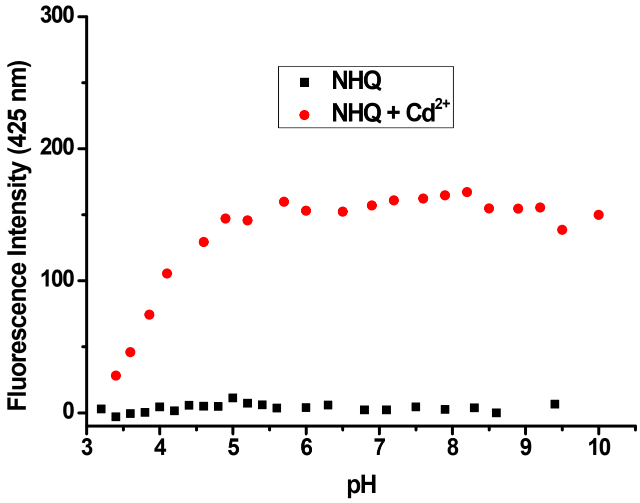


Fig. S1 The influence of pH on the fluorescence of **NHQ** (10 μM) without Cd^{2+} (black) and with 20 μM Cd^{2+} (red) in water, the pH of the solution was adjusted by adding 10% $HClO_4$ or 2 M NaOH. Excitation was performed at 310 nm.

2. UV-Vis absorption titration spectra of NHQ with Cd^{2+} in Tris-HCl

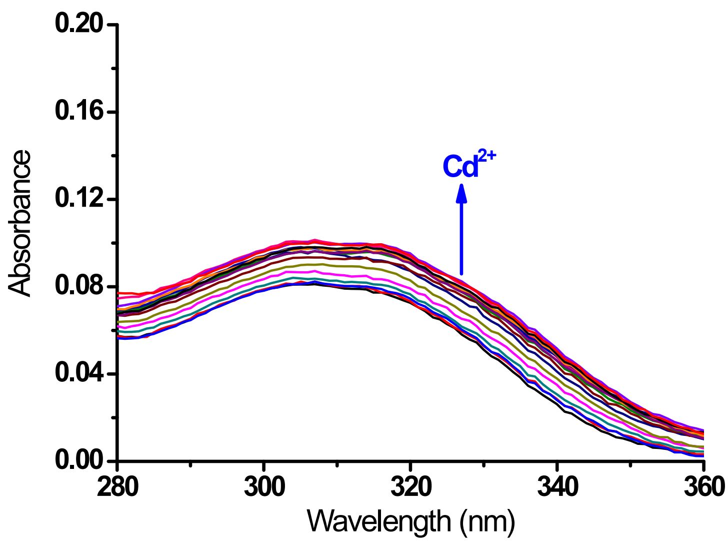


Fig. S2 UV-Vis absorption spectra of **NHQ** (10 μM) upon addition of Cd^{2+} (0-15 μM) in Tris-HCl (20 mM, pH 7.4).

3. UV-Vis absorption spectra of NHQ with various metal ions in Tris-HCl

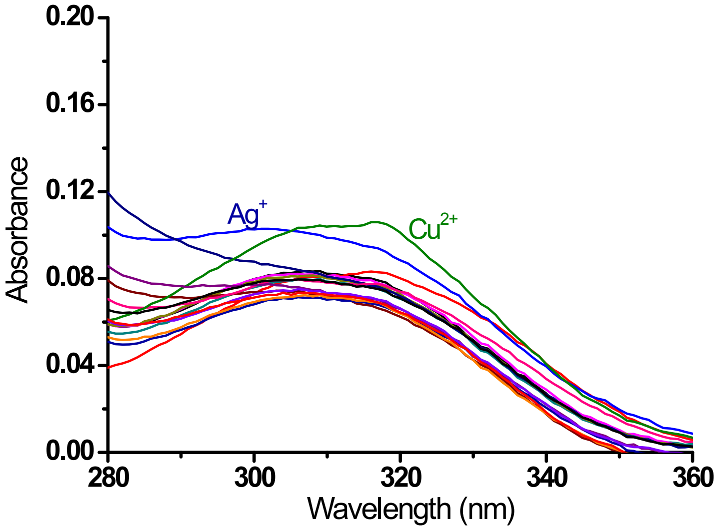


Fig. S3 UV-Vis absorption spectra of **NHQ** (10 μM) in the presence of various metal ions (20 μM) in Tris-HCl (20 mM, pH 7.4).

4. The competition experiment of NHQ for Cd^{2+} in Tris

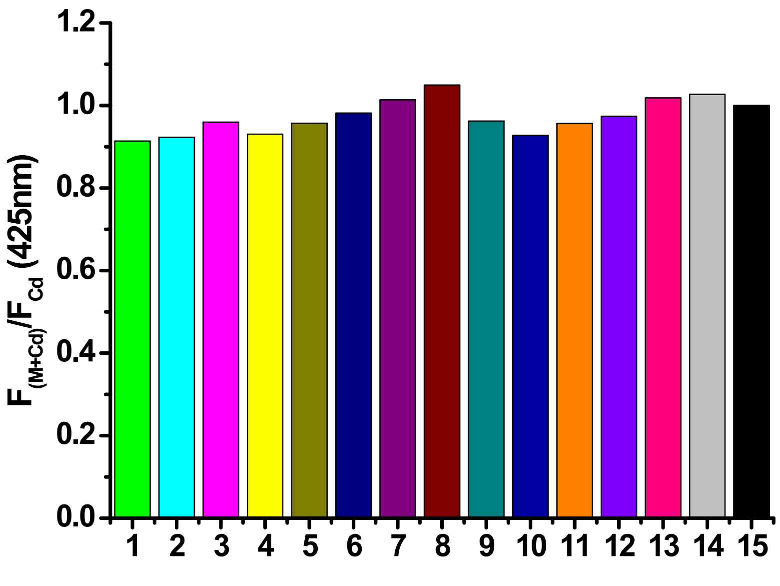


Fig. S4 Fluorescence intensity ratio of **NHQ** (10 μM) in the presence of 20 μM of metal ion and 20 μM of Cd^{2+} various **NHQ** (10 μM) in the presence of 20 μM of Cd^{2+} in Tris-HCl (20 mM, pH 7.4). 1, Co^{2+}; 2, Ag^{+}; 3, Mg^{2+}; 4, Pb^{2+}; 5, Ni^{+}; 6, Mn^{2+}; 7, Na^{+}; 8, Hg^{2+}; 9, Cu^{2+}; 10, Li^{+}; 11, Fe^{2+}; 12, Ba^{2+}; 13, Al^{3+}; 14, Zn^{2+}; 15, Cd^{2+}. $\lambda ex = 302$ nm

5. Fluorescence titration spectral of NHQ with Cd^{2+} in PBS

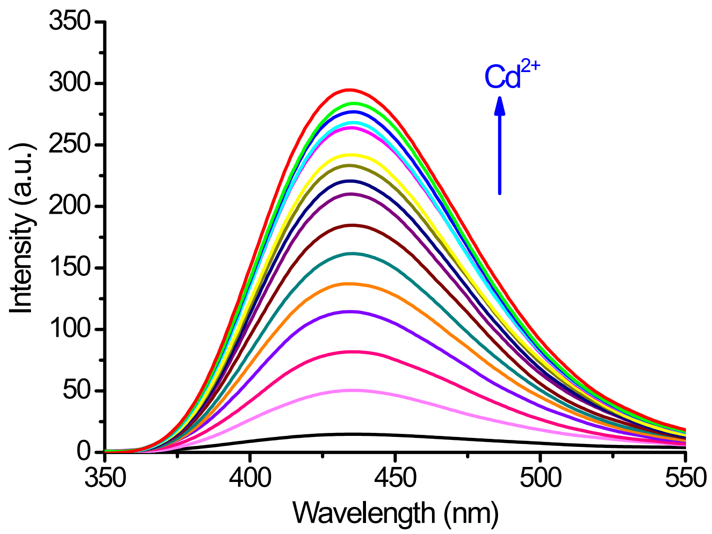


Fig. S5 Fluorescence titration spectra of **NHQ** (10 μM) upon addition of Cd^{2+} (0-15 μM) in PBS (20 mM, pH 7.4). Excitation was performed at 310 nm.

6. Cd^{2+} concentration-dependent fluorescence intensity changes of NHQ in PBS

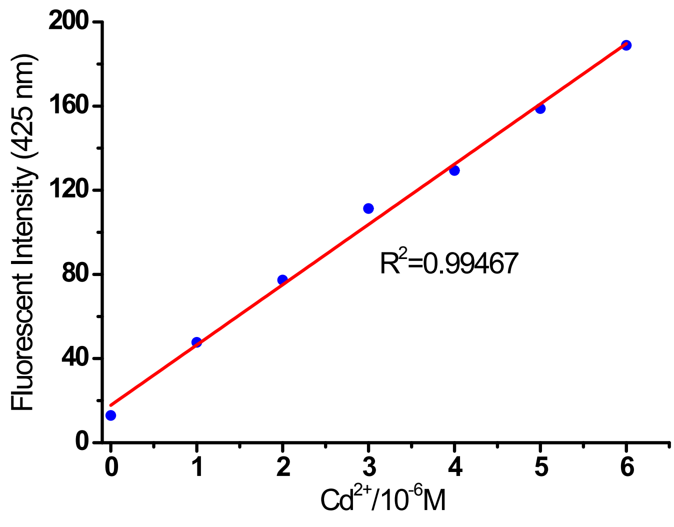


Fig. S6 Cd2+ concentration-dependent fluorescence intensity changes of **NHQ** in PBS (20 mM, pH 7.4). Concentrations of 0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0 μM of Cd2+ were added.

Detection Limit in PBS: The limit of detection of **NHQ** toward Cd^{2+} in PBS was calculated to be 3.261×10^{-7} M

7. UV-Vis absorption titration spectra of NHQ with Cd^{2+} in PBS

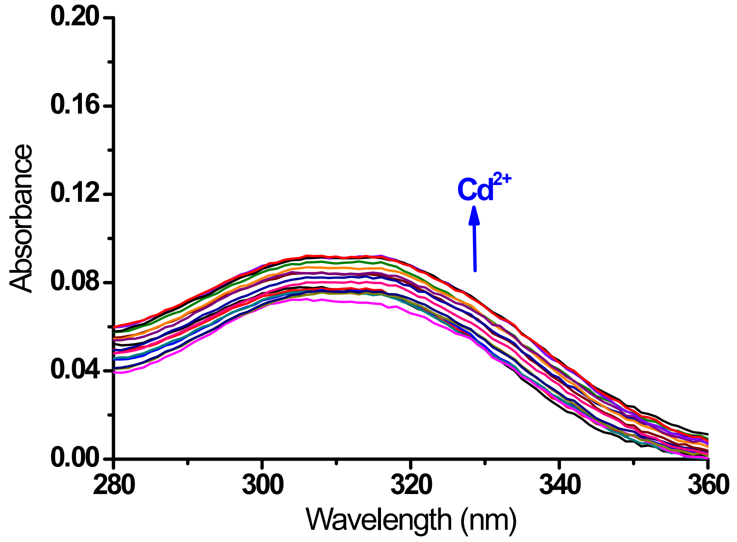


Fig. S7 UV-Vis absorption spectra of **NHQ** (10 μM) upon addition of Cd^{2+} (0-15 μM) in PBS (20 mM, pH 7.4).

8. UV-Vis absorption spectra of NHQ with various metal ions in PBS

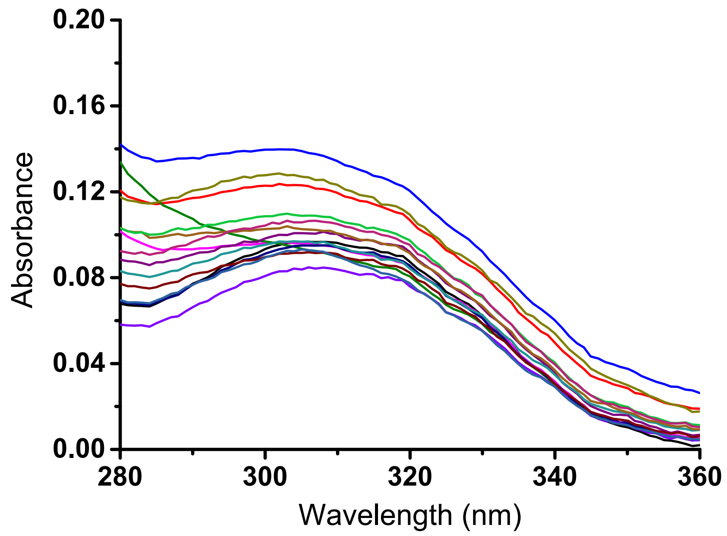


Fig. S8 UV-Vis absorption spectra of **NHQ** (10 μM) in the presence of various metal ions (20 μM) in PBS (20 mM, pH 7.4)

9. The competition experiment of NHQ for Cd^{2+} in PBS

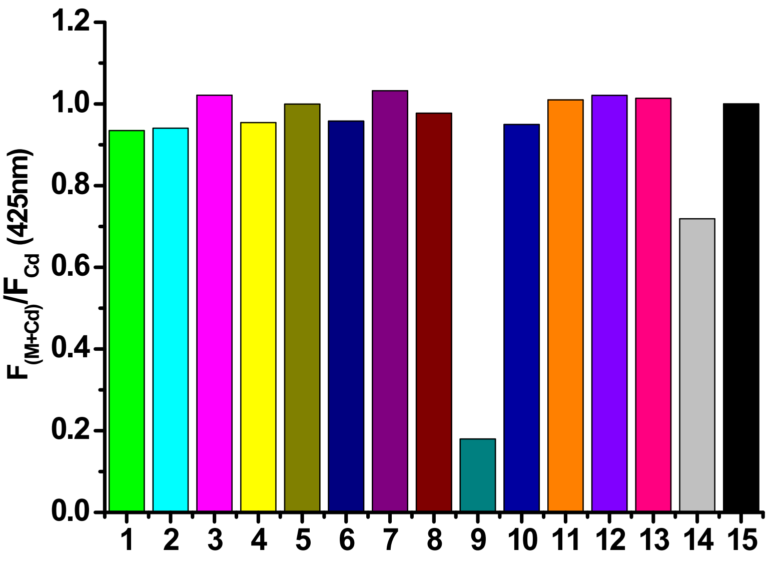


Fig. S9 Fluorescence intensity ratio of **NHQ** (10 μM) in the presence of 20 μM of metal ion and 20 μM of Cd^{2+} various **NHQ** (10 μM) in the presence of 20 μM of Cd^{2+} in PBS (20 mM, pH 7.4). 1, Co^{2+}; 2, Ag^{+}; 3, Mg^{2+}; 4, Pb^{2+}; 5, Ni^{+}; 6, Mn^{2+}; 7, Na^{+}; 8, Hg^{2+}; 9, Cu^{2+}; 10, Li^{+}; 11, Fe^{2+}; 12, Ba^{2+}; 13, Al^{3+}; 14, Zn^{2+}; 15, Cd^{2+}. λex = 310 nm.

10. Fluorescence titration spectral of NHQ with Cd^{2+} in HEPES

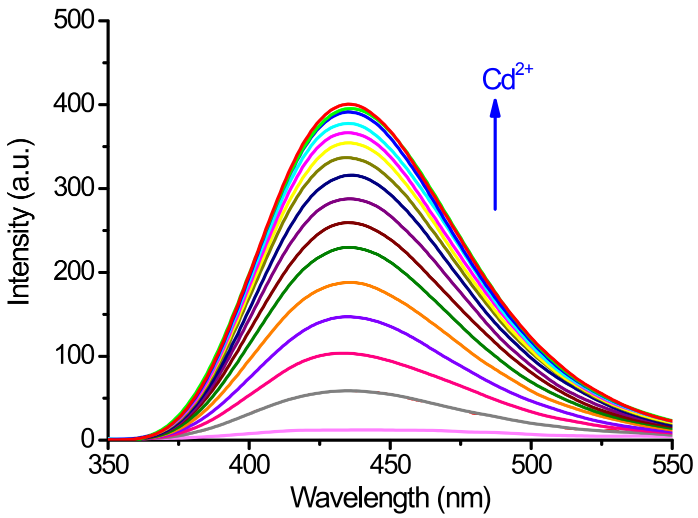


Fig. S10 Fluorescence titration spectra of **NHQ** (10 μM) upon addition of Cd^{2+} (0-15 μM) in HEPES (20 mM, pH 7.4). Excitation was performed at 310 nm.

11. Cd^{2+} concentration-dependent fluorescence intensity changes of NHQ in HEPES

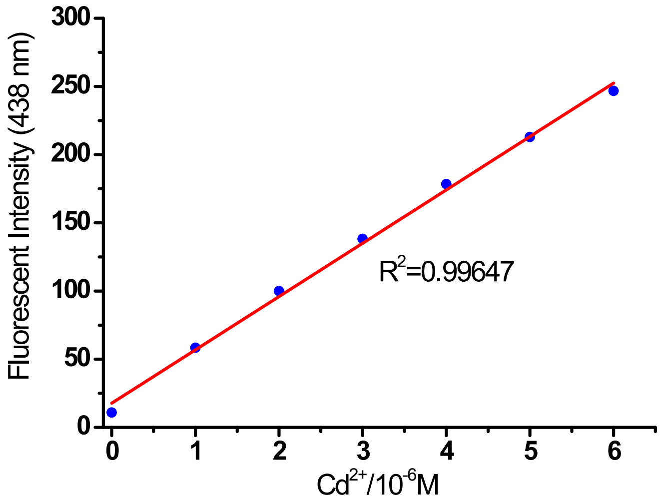


Fig. S11 Cd2+ concentration-dependent fluorescence intensity changes of **NHQ** in HEPES (20 mM, pH 7.4). Concentrations of 0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0 μM of Cd2+ were added.

Detection Limit in HEPES: The limit of detection of **NHQ** toward Cd^{2+} in HEPES was calculated to be 2.389×10^{-7} M

12. UV-Vis absorption titration spectra of NHQ with Cd^{2+} in HEPES

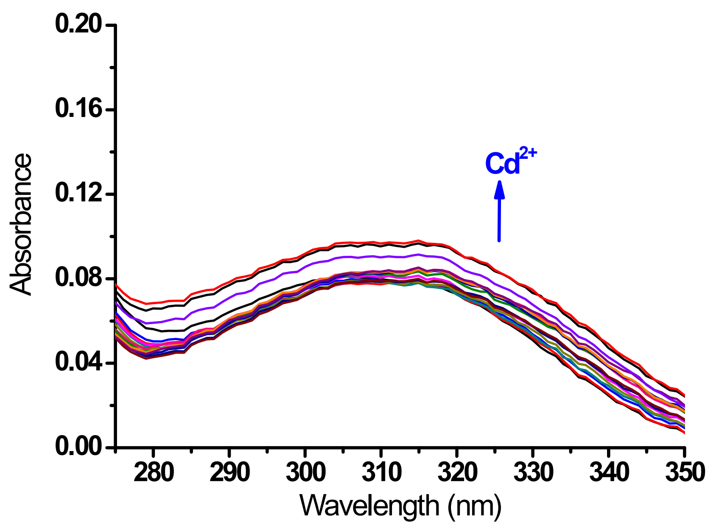


Fig. S12 UV-Vis absorption spectra of **NHQ** (10 μM) upon addition of Cd^{2+} (0-15 μM) in HEPES (20 mM, pH 7.4).

13. UV-Vis absorption spectra of NHQ with various metal ions in HEPES

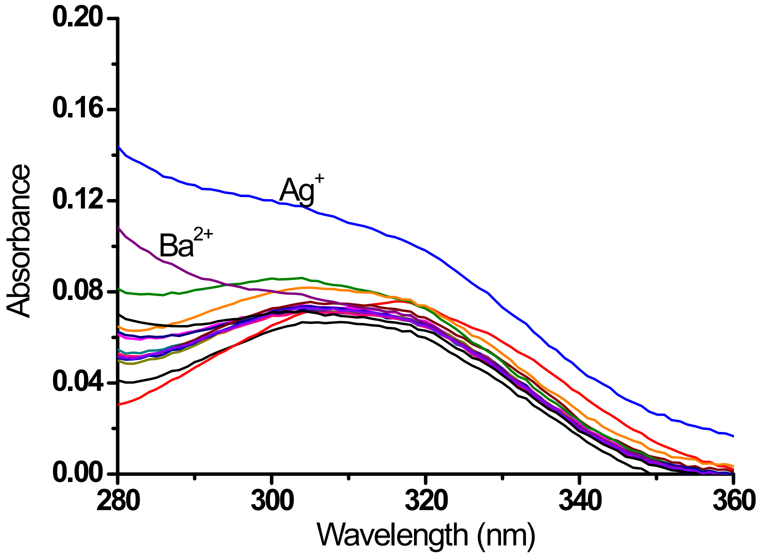


Fig. S13 UV-Vis absorption spectra of **NHQ** (10 μM) in the presence of various metal ions (20 μM) in HEPES (20 mM, pH 7.4)

14. The competition experiment of NHQ for Cd^{2+} in HEPES

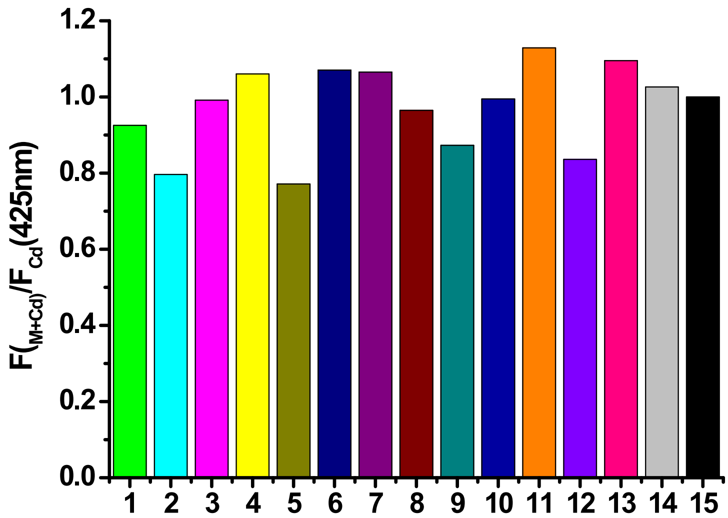


Fig. S14 Fluorescence intensity ratio of **NHQ** (10 μM) in the presence of 20 μM of metal ion and 20 μM of Cd^{2+} various **NHQ** (10 μM) in the presence of 20 μM of Cd^{2+} in HEPES (20 mM, pH 7.4). 1, Co^{2+}; 2, Ag^{+}; 3, Mg^{2+}; 4, Pb^{2+}; 5, Ni^{+}; 6, Mn^{2+}; 7, Na^{+}; 8, Hg^{2+}; 9, Cu^{2+}; 10, Li^{+}; 11, Fe^{2+}; 12, Ba^{2+}; 13, Al^{3+}; 14, Zn^{2+}; 15, Cd^{2+}. λex = 310 nm.

15. Fluorescence titration spectral of NHQ with Cd^{2+} in pure water

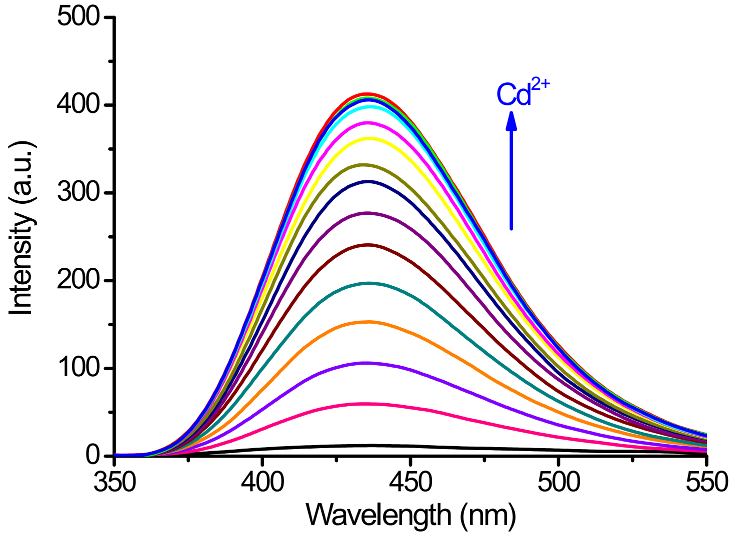


Fig. S15 Fluorescence titration spectra of **NHQ** (10 μM) upon addition of Cd^{2+} (0-15 μM) in pure water. Excitation was performed at 310 nm.

16. Cd^{2+} concentration-dependent fluorescence intensity changes of NHQ in pure water

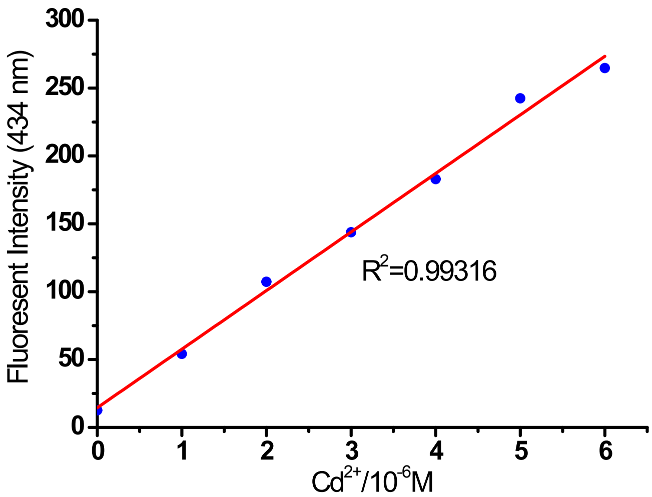


Fig. S16 Cd2+ concentration-dependent fluorescence intensity changes of **NHQ** in pure water. Concentrations of 0, 1.0, 2.0, 3.0, 4.0, 5.0, 6.0 μM of Cd2+ were added.

Detection Limit in water: The limit of detection of **NHQ** toward Cd^{2+} in pure water was calculated to be 2.165×10^{-7} M

17. UV-Vis absorption titration spectra of NHQ with Cd^{2+} in pure water

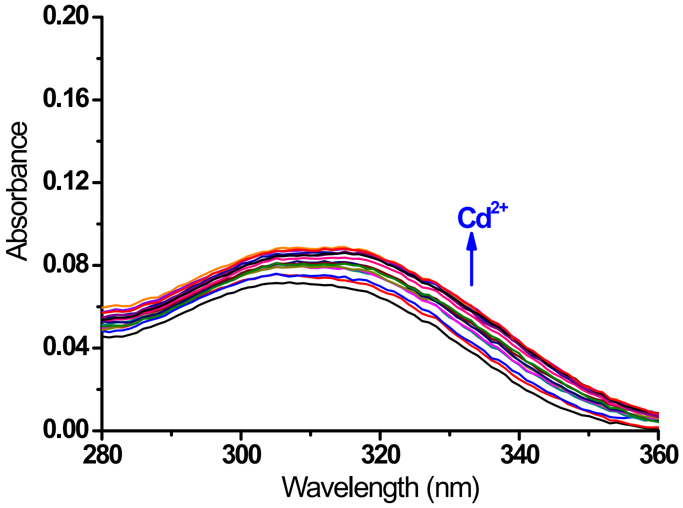


Fig. S17 UV-Vis absorption spectra of **NHQ** (10 μM) upon addition of Cd^{2+} (0-15 μM) in pure water.

18. UV-Vis absorption spectra of NHQ with various metal ions in pure water

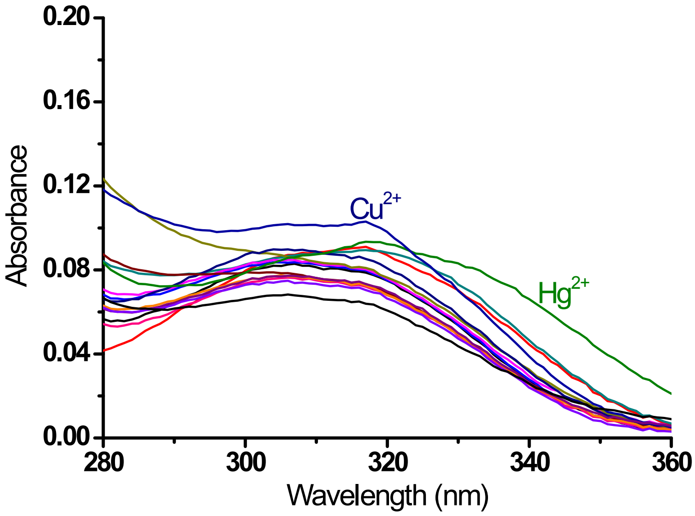


Fig. S18 UV-Vis absorption spectra of **NHQ** (10 μM) in the presence of various metal ions (20 μM) in pure water.

19. The competition experiment of NHQ for Cd^{2+} in pure water

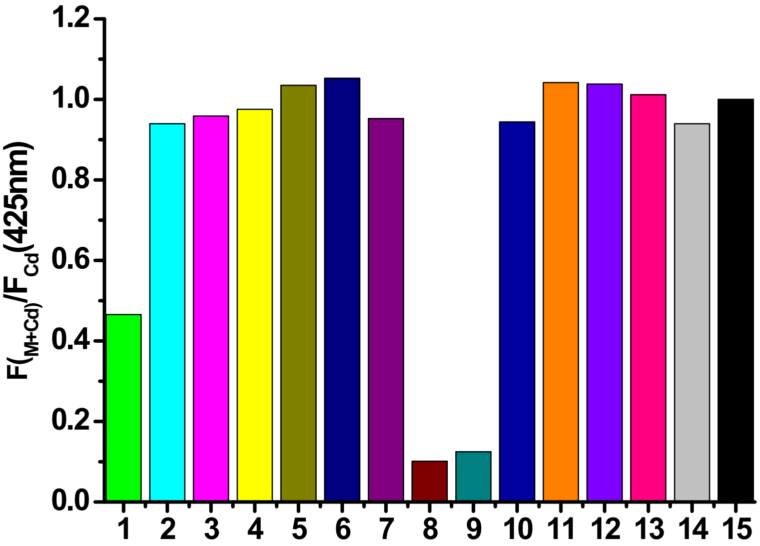


Fig. S19 Fluorescence intensity ratio of **NHQ** (10 μM) in the presence of 20 μM of metal ion and 20 μM of Cd^{2+} various **NHQ** (10 μM) in the presence of 20 μM of Cd^{2+} in pure water. 1, Co^{2+}; 2, Ag^{+}; 3, Mg^{2+}; 4, Pb^{2+}; 5, Ni^{+}; 6, Mn^{2+}; 7, Na^{+}; 8, Hg^{2+}; 9, Cu^{2+}; 10, Li^{+}; 11, Fe^{2+}; 12, Ba^{2+}; 13, Al^{3+}; 14, Zn^{2+}; 15, Cd^{2+}. λex = 310 nm.

20. Selected bond lengths (Å) and angles (deg) for $C_{27}H_{23}N_3O_4CdCl_2$

Table S1 Selected bond lengths (Å) and angles (deg) for $C_{27}H_{23}N_3O_4CdCl_2$

Bond Lengths (Å)					
Cd1-N1	2.365(5)	Cd1-N2	2.372(5)	Cd1-N3	2.392(5)
Cd1-O3	2.518(4)	Cd1-O2	2.531(4)	Cd1-Cl1	2.553(2)
Cd1-Cl2	2.711(2)				
Bond Angles (deg)					
N1-Cd1-N2	128.00(17)	N1-Cd1-N3	99.26(16)	N2-Cd1-N3	131.80(17)
N1-Cd1-O3	153.35(15)	N2-Cd1-O3	66.96(15)	N3-Cd1-O3	65.83(14)
N1-Cd1-O2	64.86(14)	N2-Cd1-O2	66.29(15)	N3-Cd1-O2	160.79(14)
O3-Cd1-O2	133.04(13)	N1-Cd1-Cl1	98.74(13)	N2-Cd1-Cl1	91.79(12)
N3-Cd1-Cl1	89.53(13)	O3-Cd1-Cl1	102.90(11)	O2-Cd1-Cl1	82.74(11)
N1-Cd1-Cl2	82.95(13)	N2-Cd1-Cl2	89.09(13)	N3-Cd1-Cl2	87.75(13)
O3-Cd1-Cl2	74.81(11)	O2-Cd1-Cl2	100.24(11)	Cl1-Cd1-Cl2	177.00(6)

21. The ^1H NMR spectra of NHQ upon addition of Cd^{2+}

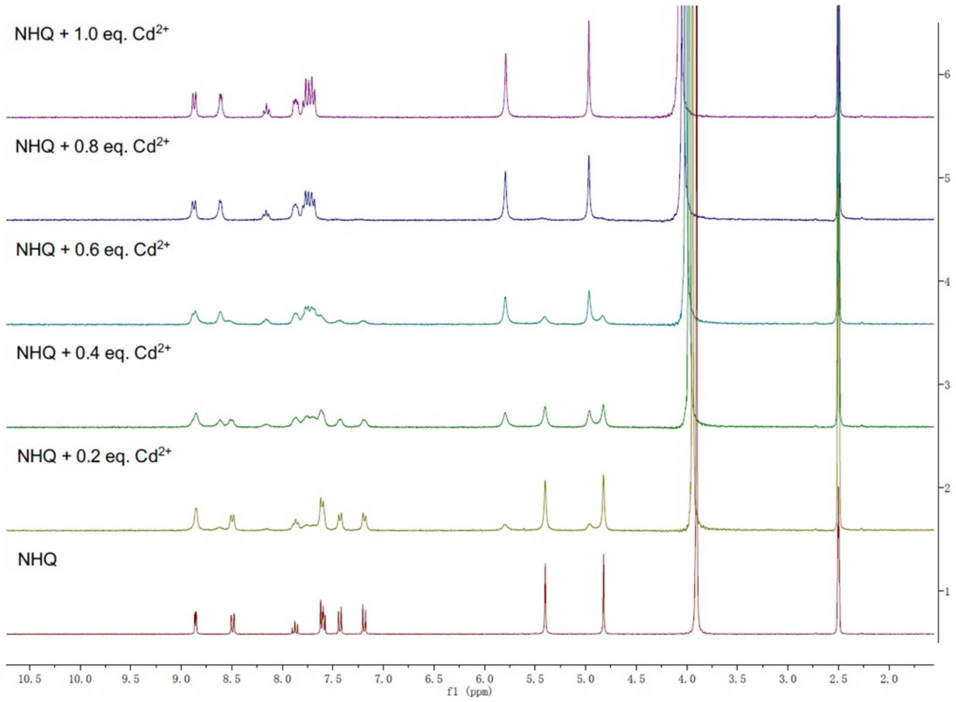


Fig. S20 The partial ^1H NMR spectra of **NHQ** upon addition of Cd^{2+} in DMSO-d_6/D_2O (5:1, v/v).

22. The ESI-MS of complex NHQ/Cd^{2+}

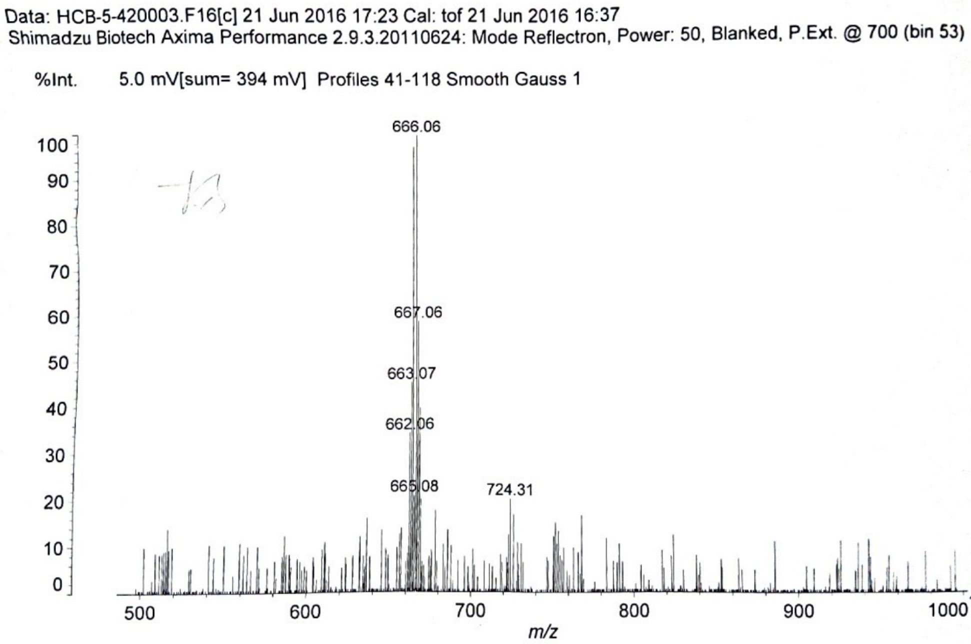
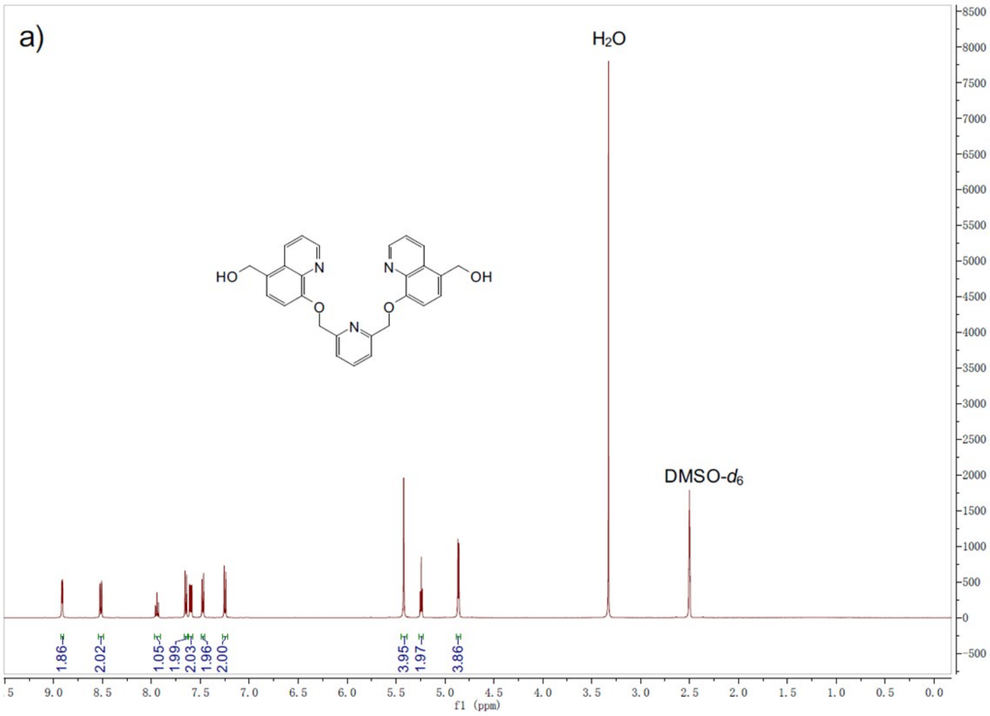


Fig. S21 The ESI-MS of complex **NHQ** and $Cd(ClO_4)_2$.

23. The 1H NMR spectrum and 13C NMR spectrum of probe NHQ



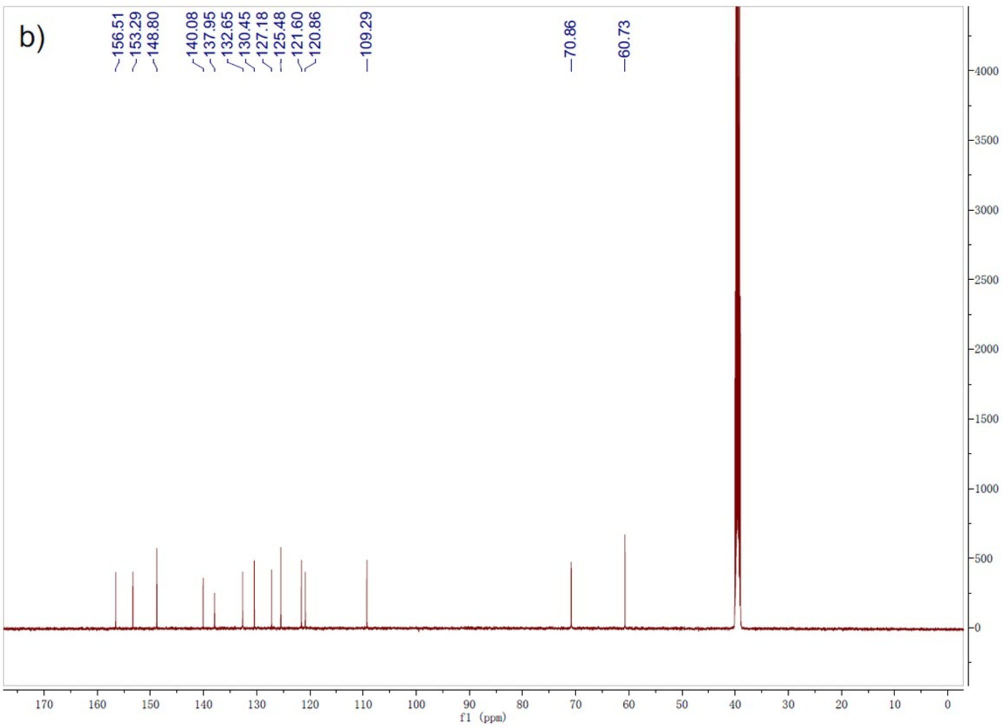


Fig. S22 The ^1H NMR spectrum (a) and ^{13}C NMR spectrum (b) of probe **NHQ** in DMSO-d_6.

24. The ESI-MS of probe NHQ

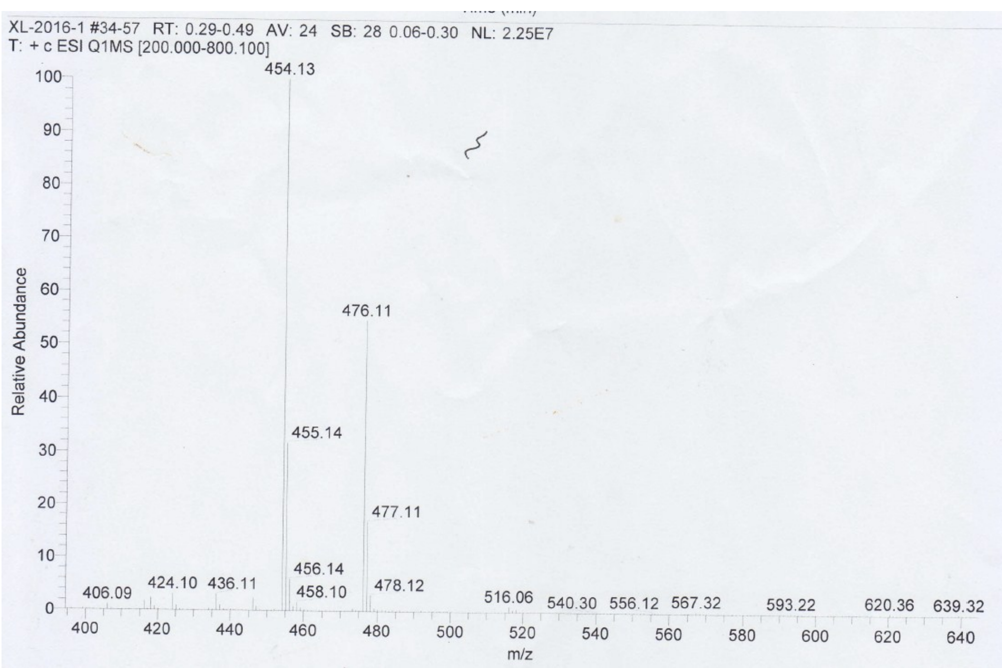


Fig. S23 The ESI-MS of probe **NHQ**.