Supporting Information for

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

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

![Fluorescence Intensity vs pH](image)

**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

![Absorbance vs Wavelength](image)

**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

![Absorption spectra](image)

**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

![Fluorescence ratio](image)

**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$^{2+}$. λ$_{ex}$ = 302 nm
5. Fluorescence titration spectral of NHQ with Cd$^{2+}$ in PBS

![Graph showing fluorescence titration spectral of NHQ with Cd$^{2+}$ in PBS](image)

**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

![Graph showing Cd$^{2+}$ concentration-dependent fluorescence intensity changes of NHQ in PBS](image)

**Fig. S6** Cd$^{2+}$ 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 Cd$^{2+}$ were added.

**Detection Limit in PBS:** The limit of detection of NHQ toward Cd$^{2+}$ in PBS was calculated to be $3.261 \times 10^{-7}$ M
7. UV-Vis absorption titration spectra of NHQ with Cd$^{2+}$ in PBS

![UV-Vis absorption spectra of NHQ with Cd$^{2+}$ in PBS](image)

**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

![UV-Vis absorption spectra of NHQ with various metal ions in PBS](image)

**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

![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.]

![Fluorescence titration spectral of NHQ with Cd$^{2+}$ in HEPES](image)

**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

![Fluorescence Intensity vs Cd\(^{2+}\) Concentration](image)

Fig. S11 Cd\(^{2+}\) 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 \(\mu\)M of Cd\(^{2+}\) were added.

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

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

![Absorption Spectra vs Wavelength](image)

Fig. S12 UV-Vis absorption spectra of NHQ (10 \(\mu\)M) upon addition of Cd\(^{2+}\) (0-15 \(\mu\)M) in HEPES (20 mM, pH 7.4).
13. UV-Vis absorption spectra of NHQ with various metal ions in HEPES

![UV-Vis absorption spectra of NHQ](image)

*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$^{2+}$. $\lambda_{ex} = 310$ nm.
15. Fluorescence titration spectral of NHQ with Cd\textsuperscript{2+} in pure water

![Fluorescence titration spectra of NHQ](image)

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

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

![Fluorescence intensity changes](image)

**Fig. S16** Cd\textsuperscript{2+} 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 Cd\textsuperscript{2+} were added.

**Detection Limit in water:** The limit of detection of NHQ toward Cd\textsuperscript{2+} in pure water was calculated to be 2.165 × 10\textsuperscript{-7} M
17. UV-Vis absorption titration spectra of NHQ with Cd$^{2+}$ in pure water

![Graph showing 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

![Graph showing 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](#)

**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$^{2+}$. $\lambda_{ex} = 310$ nm.

20. Selected bond lengths (Å) and angles (deg) for C$_{27}$H$_{23}$N$_{3}$O$_{4}$CdCl$_{2}$

**Table S1** Selected bond lengths (Å) and angles (deg) for C$_{27}$H$_{23}$N$_{3}$O$_{4}$CdCl$_{2}$

<table>
<thead>
<tr>
<th>Bond Lengths (Å)</th>
<th>Bond Angles (deg)</th>
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<tr>
<td>Cd1-N1</td>
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<td>Cd1-O3</td>
<td>2.518(4)</td>
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<td>Cd1-Cl2</td>
<td>2.711(2)</td>
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21. The $^1$H NMR spectra of NHQ upon addition of Cd$^{2+}$

![NMR spectra image]

**Fig. S20** The partial $^1$H NMR spectra of NHQ upon addition of Cd$^{2+}$ in DMSO-$_d_6$/D$_2$O (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 $^1$H 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.