Electronic Supplementary Material

for

A Fluorescent and Colorimetric Probe based on Naphthalene Diimide and High Sensitivity towards Copper Ions as Test Strips

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Table S1. Performance compared with available Cu^{2+} probes.

<table>
<thead>
<tr>
<th>Ligand name</th>
<th>Fluorescence modes</th>
<th>Detection limit</th>
<th>Fluorophore</th>
<th>Issues</th>
</tr>
</thead>
<tbody>
<tr>
<td>L1</td>
<td>Quenching, $\lambda_{ex}/\lambda_{em}$=341nm/393 nm</td>
<td>2.48 $\mu$M</td>
<td>Salicylaldehyde derivative</td>
<td>Also complex with Fe^{2+}, Fe^{3+}</td>
</tr>
<tr>
<td>L2</td>
<td>Enhancement, $\lambda_{ex}/\lambda_{em}$=440 nm/510 nm</td>
<td>28 ppb</td>
<td></td>
<td>Also complexes with Co^{2+}, Hg^{2+}</td>
</tr>
</tbody>
</table>
Enhancement

$\lambda_{ex}/\lambda_{em}=367$

$0.058 \mu M$ Coumarin derivative
Also complexes with $\text{Hg}^{2+}$ (response time $= 1h$)

Quenching

$\lambda_{ex}/\lambda_{em}=420$

$1.96 \mu M$ Coumarin derivative

Enhancement

$\lambda_{ex}/\lambda_{em}=552$

$126 \text{ ppb}$ Rhodamine derivative
Also complexes with $\text{Zn}^{2+}$

Enhancement

$\lambda_{ex}/\lambda_{em}=460$

$0.023 \mu M$ DCM derivative
Response time $= 40$ min

Enhancement

$\lambda_{ex}/\lambda_{em}=470$ nm

$55 \text{ nM}$ Fluorescein derivative
Response time $= 1$ min

Quenching

$\lambda_{ex}/\lambda_{em}=470$ nm

$0.84 \mu M$
Fig. S1 Time-dependent quenching upon addition of a Cu ion source. The excited wavelength was 605 nm.

Fig. S2 The fluorescence intensity of NDI-Py in solution (concentration: $1 \times 10^{-5}$ mol/L) with increasing scan (0–3600 s). Excitation wavelength: 605 nm.
**Fig. S3** The UV-visible spectra of NDI-Py in acetone (20 µM) towards 1.0 equiv. of various metal ions.

**Fig. S4** The changes of fluorescence intensity of NDI-Py (10 µM in acetone) at 638 nm with 10 equiv of different anions. (1) Blank; (2) F⁻; (3) Cl⁻; (4) I⁻; (5) Br⁻; (6) ClO₃⁻; (7) CO₃²⁻; (8) HCO₃⁻; (9) HSO₃⁻; (10) S₂O₃²⁻; (11) S₂O₅²⁻; (12) SO₃²⁻; (13) SO₄²⁻; (14) NO₂⁻; (15) NO₃⁻.
Fig. S5 Fluorescence spectra of NDI-Py (10 μM in acetone) with the addition of different metal ions (1 equiv.) at the same time.

Fig. S6 (A) The changes of fluorescence intensity of NDI-Py in acetone with different HEPES buffer (10 μM, pH=7.0) contents; (B) Relationship between the HEPES buffer (10 μM, pH=7.0) contents and the corresponding fluorescence intensity and maximum emission wavelength of NDI-Py in acetone/HEPES mixed solvent
Fig. S7 Fluorescence spectra profiles of NDI-Py in acetone and HEPES solution (v/v: 7/3) (10 μM) towards 1.0 equiv of various metal ions. Inset: fluorescence photographs of compound NDI-Py with various metal ions: A) Cu$^{2+}$, B) Hg$^{2+}$, C) Ag$^{+}$, D) Al$^{3+}$, E) Na$^+$, F) K$^+$, G) Ca$^{2+}$, H) Mg$^{2+}$, I) Zn$^{2+}$, J) Fe$^{3+}$, K) Fe$^{2+}$, L) Ba$^{2+}$, M) Mn$^{2+}$, N) Pb$^{2+}$, O) Co$^{2+}$, P) Li$^+$, Q) Cr$^{3+}$, R) Cd$^{2+}$, S) Ni$^{2+}$, T) NDI-Py

Fig. S8 Fluorescence spectra profiles of NDI-Py in acetone and HEPES solution (V/V: 7/3) (10 μM) towards 1 equiv. of copper ions in the presence of the same amount of
other metal ions. 1) NDI-Py, 2) Hg$^{2+}$, 3) Ag$^+$, 4) Al$^{3+}$, 5) Na$^+$, 6) K$^+$, 7) Ca$^{2+}$, 8) Mg$^{2+}$, 9) Zn$^{2+}$, 10) Fe$^{3+}$, 11) Fe$^{2+}$, 12) Ba$^{2+}$, 13) Mn$^{2+}$, 14) Pb$^{2+}$, 15) Co$^{2+}$, 16) Li$^+$, 17) Cr$^{3+}$, 18) Cd$^{2+}$, 19) Ni$^{2+}$. The magenta bars represent the relative fluorescence intensities of NDI-Py with various metal ions. The navy bars represent the relative fluorescence intensities of NDI-Py towards copper ions in the presence of other competing metal ions.

![Absorption graph](image)

**Fig. S9** The changes of absorption of NDI-Py at 663 nm in acetone (20 μM).

![Job's plot graphs](image)

**Fig. S10 (A)** Job’s plot of NDI-Py and copper ions ([NDI-Py] + [Cu$^{2+}$] = 40 μM) in acetone by UV-vis spectra, where the absorption at 663 nm was plotted against the mole fraction of [Cu$^{2+}$/[NDI-Py]+Cu$^{2+}$]. (B) Job’s plot of NDI-Py and copper ions ([NDI-Py] + [Cu$^{2+}$] = 40 μM) in acetone by fluorescence spectra, where the fluorescence intensity at 638 nm was plotted against the mole fraction of [Cu$^{2+}$/[NDI-Py]+Cu$^{2+}$].
**Fig. S11** ESI-MS spectrum of NDI-Py with copper ions.

**Fig. S12** Fluorescence titration curve of NDI-Py (2.0 μM) in acetone with different concentrations of copper ions.
Fig. S13 The changes of fluorescence signal with different concentrations of copper ions

Fig. S14 The changes of fluorescence intensity of NDI-Py in the presence and absence of Cu^{2+} with variation of pH values.
Fig. S15 The $^1$H NMR spectrum of compound 2

Fig.S16 The $^1$H NMR spectrum of compound 3
Fig.S17 The $^{13}$C NMR spectrum of compound 3.
Fig. S18 The $^1$H NMR spectrum of NDI-Py

Fig. S19 The $^{13}$C NMR spectrum of NDI-Py
Fig. 20 The HRMS spectrum of NDI-Py