Supplementary Data

For

A novel near-infrared and naked-eyes turn on fluorescent probe for detection of biothiols with a large stokes shift and its application in living cells

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<table>
<thead>
<tr>
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<th>Probe</th>
<th>Solvent (pH=7.4)</th>
<th>Dose of Cys (eq.)</th>
<th>Time (min)</th>
<th>Stokes shift (nm)</th>
<th>Naked eyes</th>
<th>Detection Limit (μM)</th>
<th>Reference</th>
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<td>Hcy</td>
<td>GSH</td>
<td>Ref.</td>
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</table>

**Table S1.** Some similar functionalized probes for the detection of biothiols
Figure S1. $^1$H NMR (400 MHz) spectrum of compound 1 in DMSO-$d_6$.

Figure S2. $^{13}$C NMR (100 MHz) spectrum of compound 1 in DMSO-$d_6$. 
Figure S3. $^1$H NMR (400 MHz) spectrum of HDM in DMSO-$d_6$.

Figure S4. $^{13}$C NMR (100 MHz) spectrum of HDM in DMSO-$d_6$. 
Figure S5. $^1$H NMR (400 MHz) spectrum of probe DDND in DMSO-$d_6$.

Figure S6. $^{13}$C NMR (100 MHz) spectrum of probe DDND in DMSO-$d_6$. 
Figure S7. HRMS (ESI⁺) spectrum of probe DDND.

Figure 8. Fluorescence spectra of DDND by itself (10 μM, gray line), and DDNA (10 μM) in the presence of Cys (1 mM, red line), Hcy (1 mM, black line) and GSH (1 mM, blue line). Ex=492 nm.
Figure S9. (a) Fluorescence titration of DDND (10 μM) upon addition of Hcy (0-30 μM). Ex = 492 nm, slit: 5.0 nm/5.0 nm; (b) Stand curve of F/F₀ at 623 nm versus Hcy concentration (from 0 to 16 μM). F₀ and F are the fluorescence intensity in the absence and presence of Hcy, respectively. Ex = 492 nm, slit: 5.0 nm/5.0 nm.

Figure S10. (a) Fluorescence titration of DDND (10 μM) upon addition of GSH (0-30 μM). Ex = 492 nm, slit: 5.0 nm/5.0 nm; (b) Stand curve of F/F₀ at 623 nm versus GSH concentration (from 0 to 16 μM). F₀ and F are the fluorescence intensity in the absence and presence of Hcy, respectively. Ex = 492 nm, slit: 5.0 nm/5.0 nm.
Figure S11. Emission color changes of probe DDND with various analytes.

Figure S12. TLC analysis of the reaction product A with the reference compound HDM and probe DDND. The TLC plate was observed under a light of 254 nm. The eluent for TLC: petroleum ether:ethyl acetate = 1:4 (v/v). This data showed that compound A was compound HDM.
**Figure S13.** $^1$H NMR spectrum analysis of product A with the reference compound HDM.

**Figure S14.** A comparison of (a) fluorescent spectra and (b) absorbance spectra of probe DDND (10 µM), compound HDM (10 µM), and the mixture of probe DDND (10 µM) + Cys (50 µM) after 15 min in PBS buffer (50% DMSO) solution.
**Figure S15.** Probe DDND with different concentration of Cys under UV irradiation (365 nm).

**Figure S16.** Viable HeLa cells after treatment with indicated concentrations of probe after 24 hours. The cell viability was observed via MTT assay.

**References**


