Supplementary Information

Highly selective fluorescent carbon dots probe of mercury(II) based on thymine-mercury(II)-thymine structure

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List of Figures

S1 Plot of the absorbance intensity at 270 nm as a function of thymine-1-acetic acid concentration in the presence of 100 μg/mL the CDs-Thy (0.1 M PBS buffer, pH 7.4). .................................................. 3

S2 (A) Fluorescence response of probe (0.1 mg/mL) in the absence (top line) and presence (bottom line) of Hg$^{2+}$ (33.3 μM), respectively. (B) Reaction-time profiles of probe (0.1 mg/mL) in the presence of Hg$^{2+}$ (1, 4, 30, and 50 μM). The fluorescence intensities at 441 nm were monitored in aqueous solution (0.2 M PBS buffer, pH 7.4) ($\lambda_{ex} = 354$ nm, slit: 5/5 nm). ............................................. 4

S3 Linear plots of the fluorescence intensities of CDs-Thy (33.3 μg/mL) upon addition of Hg$^{2+}$ (0, 0.1, 0.2, 0.4, 0.6, 0.8, and 1.0 μM) in PBS buffer solution (0.1 M, pH 7.4). .................................................. 6

List of Tables

S1 Fluorescence lifetimes of CDs-PEI and CDs-Thy .......................... 7
Figure S1. Plot of the absorbance intensity at 270 nm as a function of thymine-1-acetic acid concentration in the presence of 100 µg/mL the CDs-Thy (0.1 M PBS buffer, pH 7.4).
Figure S2. (A) Fluorescence response of probe (0.1 mg/mL) in the absence (top line) and presence (bottom line) of Hg$^{2+}$ (33.3 µM), respectively. (B) Reaction-time profiles of probe (0.1 mg/mL) in the presence of Hg$^{2+}$ (1, 4, 30, and 50 µM). The fluorescence intensities at 441 nm were monitored in aqueous solution (0.2 M PBS buffer, pH 7.4) ($\lambda_{ex} = 354$ nm, slit: 5/5 nm).

Fig. S2A shows the fluorescent intensities of the CDs-Thy under different pH from pH 5.8 to 8.2 in the absence and presence of Hg$^{2+}$, respectively. Without Hg$^{2+}$, the fluorescence intensity of the CDs-Thy have a slightly decrease with the increasing of pH. But the fluorescence intensities still stayed at a strong emission level. Upon addition of Hg$^{2+}$, the fluorescence spectra of CDs-Thy had a relatively weak emission and remained unaffected during this pH range. Therefore, the CDs-Thy can successfully detect Hg$^{2+}$ in the pH range from 5.8 to 8.2 and a PBS buffer (pH = 7.4) was chosen for all subsequent detection assays.

Fig. S2B shows the quenching kinetics of the CDs-Thy with different Hg$^{2+}$ concentration at different time by recording the fluorescence spectra. The dramatic fluorescence quenching was observed within less than 30 seconds when 30 µM and 30 µM Hg$^{2+}$ was introduced into the sensing system containing 0.1 mg/mL.
of the CDs-Thy, indicating that quenching kinetics was fairly fast. Moreover, the fluorescence emission was quenched to a stable state in 10 minutes even in the case of lower concentrations of Hg$^{2+}$. Thus, this sensing system could be used for the real-time monitoring of Hg$^{2+}$ in practical analysis.
Figure S3. Linear plots of the fluorescence intensities of CDs-Thy (33.3 μg/mL) upon addition of Hg$^{2+}$ (0, 0.1, 0.2, 0.4, 0.6, 0.8, and 1.0 μM) in PBS buffer solution (0.1 M, pH 7.4).
**Table S1.** Fluorescence lifetimes of CDs-PEI and CDs-Thy

<table>
<thead>
<tr>
<th>Sample</th>
<th>$\tau_1$ (ns)</th>
<th>$A_1$</th>
<th>Percent (%)</th>
<th>$\tau_2$ (ns)</th>
<th>$A_2$</th>
<th>Percent (%)</th>
<th>$\tau_{avg}$ (ns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CDs-PEI</td>
<td>2.24</td>
<td>0.017</td>
<td>11.99</td>
<td>12.16</td>
<td>0.023</td>
<td>88.01</td>
<td>10.97</td>
</tr>
<tr>
<td>CDs-Thy</td>
<td>3.81</td>
<td>0.017</td>
<td>19.27</td>
<td>11.69</td>
<td>0.023</td>
<td>80.73</td>
<td>10.17</td>
</tr>
</tbody>
</table>

$\tau_1$ and $\tau_2$ refer to the short and long lifetime, respectively.