## **Supplementary Information**

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

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**Figure S1.** Plot of the absorbance intensity at 270 nm as a function of thymine-1acetic acid concentration in the presence of 100  $\mu$ g/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<sup>2+</sup> (33.3  $\mu$ M), respectively. (B) Reaction-time profiles of probe (0.1 mg/mL) in the presence of Hg<sup>2+</sup> (1, 4, 30, and 50  $\mu$ M). 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<sup>2+</sup> concentration at different time by recording the fluorescence spectra. The dramatic fluorescence quenching was observed within less than 30 seconds when 30  $\mu$ M and 30  $\mu$ M Hg<sup>2+</sup> 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 fluoresence intensities of CDs-Thy (33.3  $\mu$ g/mL) upon addition of Hg<sup>2+</sup> (0, 0.1, 0.2, 0.4, 0.6, 0.8, and 1.0  $\mu$ M) in PBS buffer solution (0.1 M, pH 7.4).

Sample	$\tau_1$ (ns)	$A_1$	Percent (%)	$ au_2$ (ns)	$A_2$	Percent (%)	$\tau_{\rm avg}~({\rm ns})$
CDs-PEI	2.24	0.017	11.99	12.16	0.023	88.01	10.97
CDs-Thy	3.81	0.017	19.27	11.69	0.023	80.73	10.17

**Table S1.** Fluorescence lifetimes of CDs-PEI and CDs-Thy

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