

## Supplementary Materials

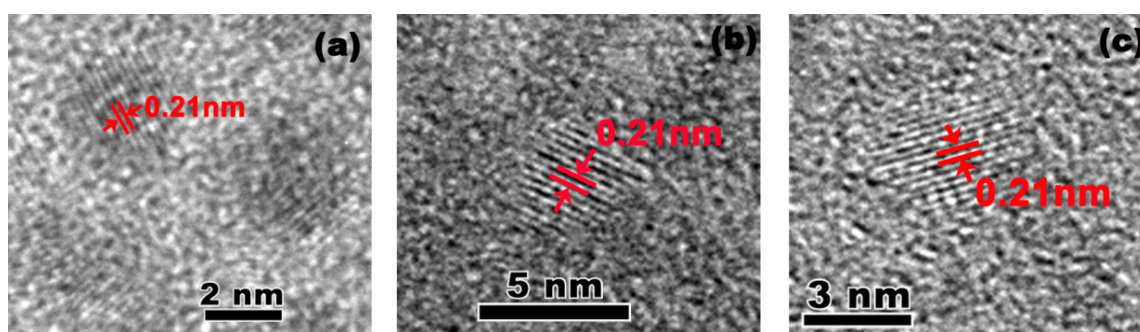


Figure S1. HRTEM images of molecule-modified CDs from S1 (a); S2 (b) and S3 (c), respectively.

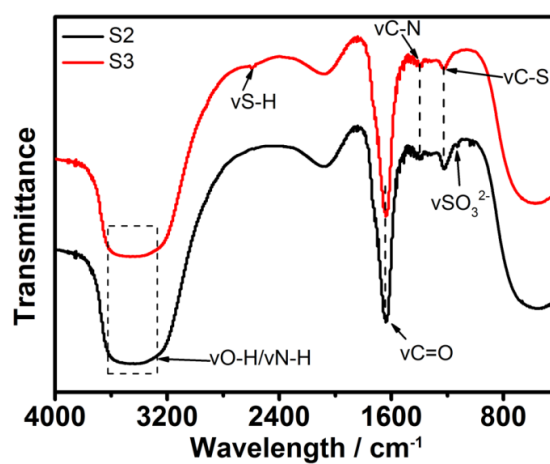


Figure S2. IR spectra of S2 and S3.

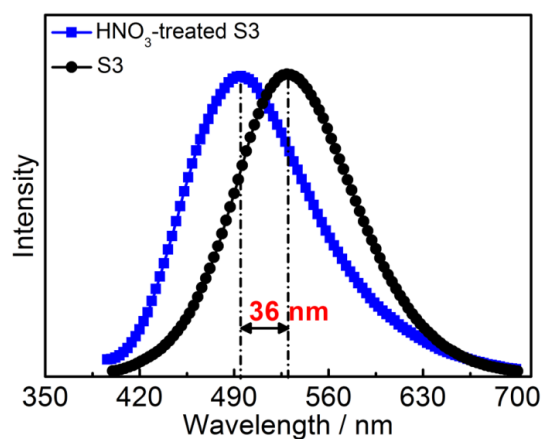
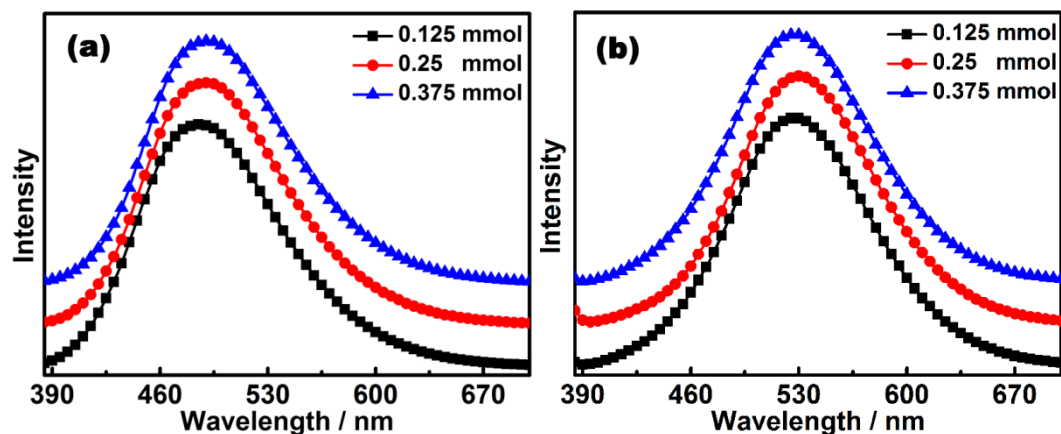
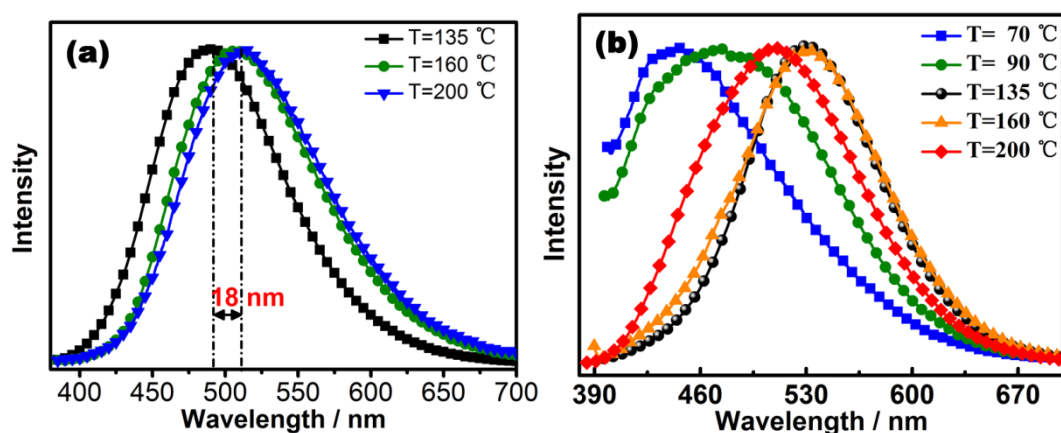


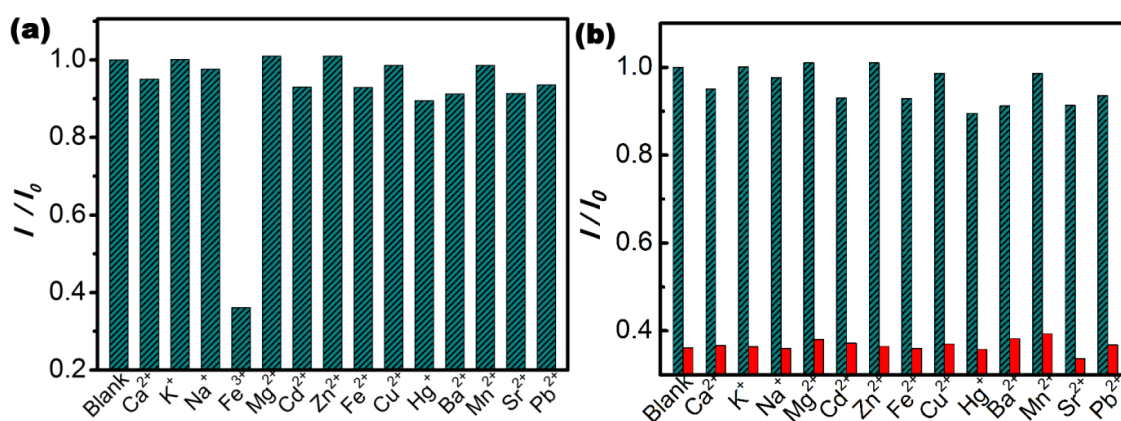
Figure S3. PL spectra of S3 and HNO<sub>3</sub>-treated S3. Here, 2.5 mL of concentrated HNO<sub>3</sub> was added in 10 mL of S3 solution. Then the mixed solution heated at 40–50 °C for 3 h under the stirring. The obtained solution was neutralized with base and then removed the excess salt and water to keep the carbon dot concentration unchanged.



**Figure S4.** PL spectra of the samples obtained by changing the amounts of sulfanilic acid (a) and 4-aminothiophenol (b) adding into the 10 mL CDs-COOH solution at the same excitation wavelength.



**Figure S5.** Effects of reaction temperature on PL properties of S2 (a) and S3 (b) at the same excitation wavelength.



**Figure S6.** (a) PL intensity ratio ( $I/I_0$ ) of the S2 in the absence and presence of different metal ions (1 mM); (b) The  $I/I_0$  comparison of S2 in the presence of  $Fe^{3+}$  ions (1 mM) upon adding different metal ions (1 mM) listed from left to right: blank,  $Ca^{2+}$ ,  $K^+$ ,  $Na^+$ ,  $Mg^{2+}$ ,  $Cd^{2+}$ ,  $Zn^{2+}$ ,  $Fe^{2+}$ ,  $Cu^{2+}$ ,  $Hg^+$ ,  $Ba^{2+}$ ,  $Mn^{2+}$ ,  $Sr^{2+}$ , and  $Pb^{2+}$ .