**Supporting Information:**

Employing the Aqueous CdTe Quantum Dots with Diversified Surface Functionalities to Discriminate Heme (Fe(II)) and Hemin (Fe(III))

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Fig. S1 pH effect on the relative PL intensity (I/I_0) of MPA- (a), TGA- (b), and TG- (c) stabilized CdTe QDs in the presence of heme (black) or hemin (red). The concentration of CdTe QDs is 0.125 mM, referring to $[Cd^{2+}]$. The concentration of heme/hemin is 12.5 μM.
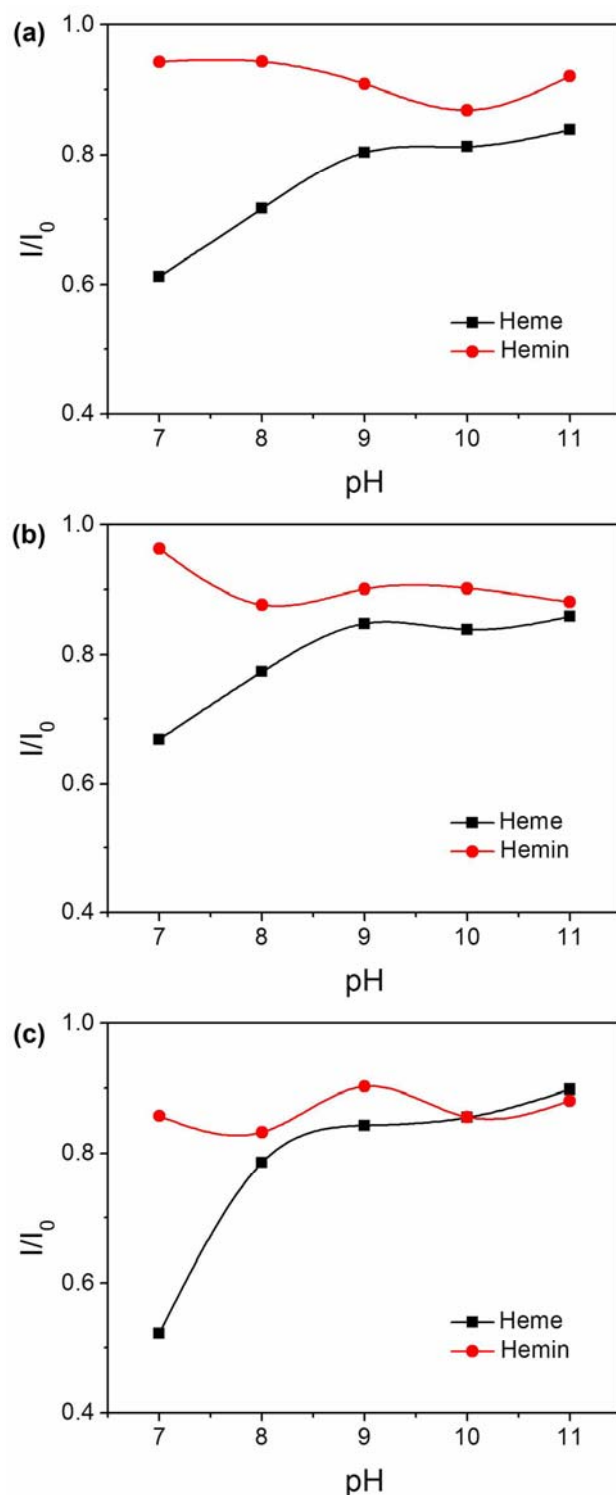
In general, with decreasing the pH, the I/I_0 in the presence of heme decreases gradually, whereas it increases for hemin. This result further confirms our consideration that the QD-carboxylate repulsion is dominant for the primary adsorption of heme/hemin and therefore the discrimination through PL quenching. In

this context, the lowered pH reduces the negative charges of both QDs and heme/hemin by carboxylate deprotonation, thus facilitating the adsorption of heme/hemin with QDs. Because heme and hemin possess different net charges, as discussed in the main text (Page 4 Line 25-36), they lead to the observed response of QD PL. In addition, the colloidal stability of QDs is worse at lower pH. Consequently, the optimum pH of 9.3 is adopted in our investigations.

Fig. S2 Relative PL intensity (I/I_0) of MPA- (a, b), TGA- (c, d), and TG- (e, f) stabilized CdTe QDs as a function of heme and hemin. The corresponding PL spectra of CdTe QDs are indicated in Fig. 3.
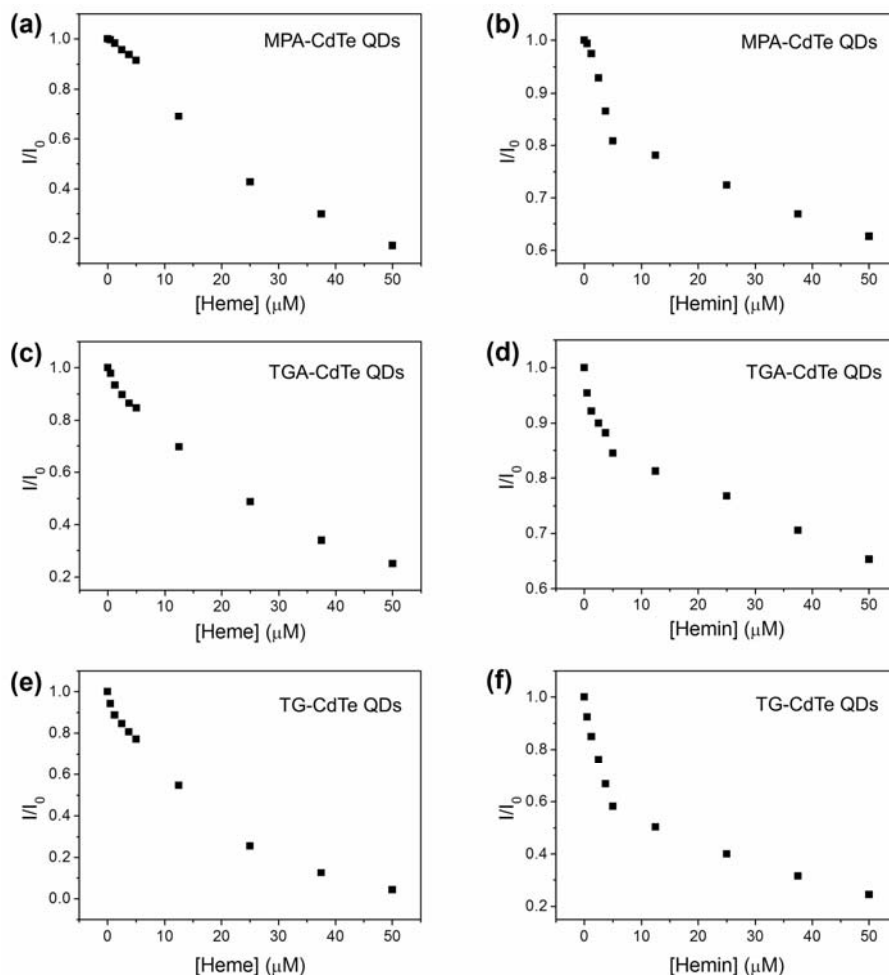
The limit of detection of Fig. 6 is evaluated using $3\sigma/S$, where σ is the standard deviation of the blank signal and the S is the slope of the calibration plot.

Fig. 6a, 4.4×10^{-7} M;
Fig. 6b, 4.3×10^{-7} M;
Fig. 6c, 1.9×10^{-7} M;
Fig. 6d, 1.8×10^{-7} M;
Fig. 6e, 2.5×10^{-7} M;
Fig. 6f, 5.7×10^{-7} M;
Fig. 6g, 2.8×10^{-7} M;
Fig. 6h, 1.8×10^{-6} M;
Fig. 6i, 9.5×10^{-8} M;
Fig. 6j, 1.0×10^{-6} M;