Electronic Supporting Information

Facile Preparation of Gadolinium(III) Chelates Functionalized Carbon Quantum Dots-based Contrast Agent for Magnetic Resonance/Fluorescence Multimodal Imaging

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1. Weight extinction coefficient of Gd(III)/CQDs

The weight extinction coefficient of Gd(III)/CQDs at 365 nm and 488 nm were measured according to Lambert-Beer law. In brief, water solutions of Gd(III)/CQDs with different mass concentration of 0.1, 0.25, 0.5, 0.8 and 1 mg·L^{-1} were prepared, whose absorbances at 365 nm and 488 nm, respectively, were recorded by an UV-vis spectrophotometer (Hitachi U2001). The weight extinction coefficient was calculated through dividing the absorbance by the concentration and the cell length (1 cm). **As** shown in Figure S1, the weight extinction coefficient (*a*) of the Gd(III)/CQDs at 365 nm and 488 nm was 1.99 L·g^{-1}·cm^{-1} and 0.72 L·g^{-1}·cm^{-1}, respectively.

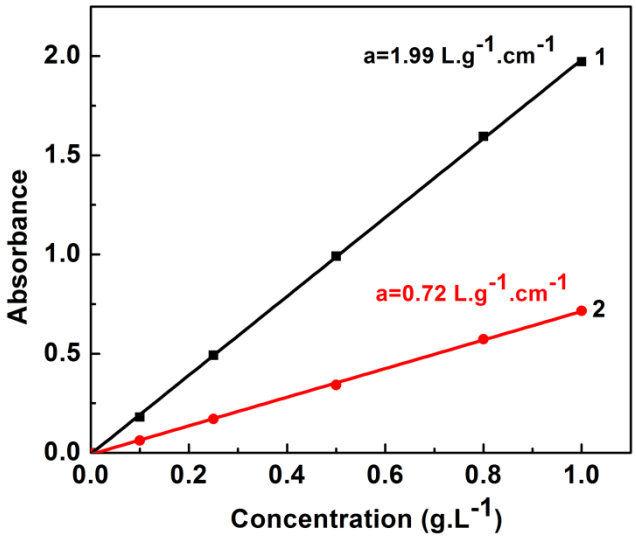

Figure S1 **Absorbances versus weight concentration of Gd(III)/CQDs prepared at 300 °C at 365nm (1) and 488 nm (2).**

2. Dispersibility of Py-GdPM, Py-Mx and the mixture of Py-GdPA and Py-Meg.

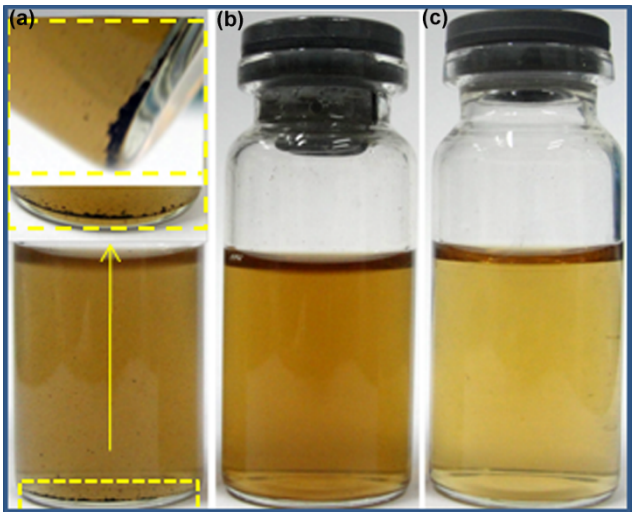

Figure S2 Water dispersion (1 mg.mL^{-1}) of the (a): mixture of Py-Meg and Py-GdPA, (b) Py-Mx, and (c) Py-GdPM (300 ^{o}C).

3. TEM images of Gd(III)/CQDs prepared at 250 ^{o}C and 300 ^{o}C, respectively.

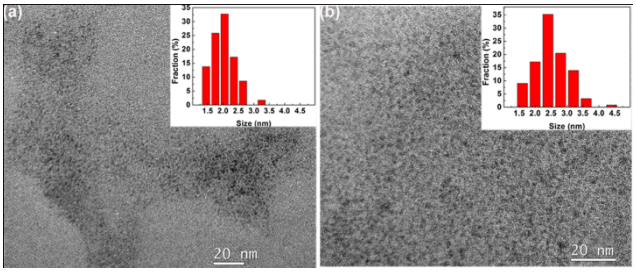

Figure S3 TEM images and size histograms of Gd(III)/CQDs prepared at (a) 250 ^{o}C and (b) 300 ^{o}C.

4. Wide-scan XPS spectra

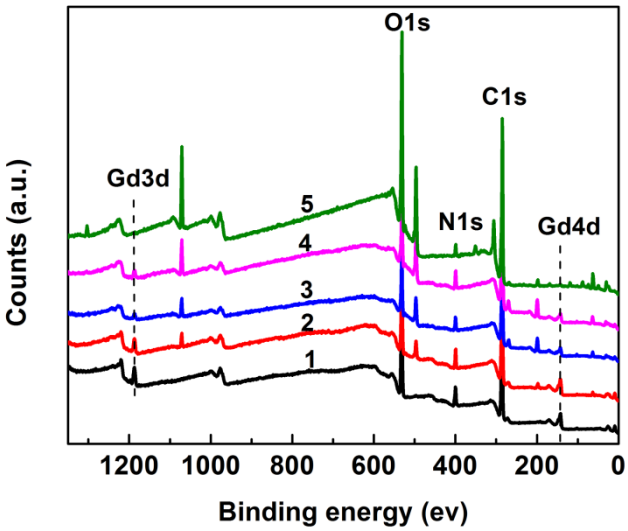

Figure S4 Wide-scan XPS spectra (1: GdPM; 2-5: Gd(III)/CQDs prepared at 250 ^{o}C, 300 ^{o}C, 350 ^{o}C and 400 ^{o}C, respectively).

5. Dialysis experiment

Two solutions (5 mL) containing Gd^{3+} at a concentration of 0.4 $mg \cdot mL^{-1}$ were prepared by dissolving gadopentetic acid and Gd(III)/CQDs into water, respectively. Each of them was dialyzed against a dialysate of 500 mL deionized water through a 1000D dialysis bag (with a pore diameter of about 1.2 nm). The concentrations of Gd^{3+} in the dialysate at different time passing through dialysis bag during dialysis were detected by an inductively coupled plasma optical emission spectrometer (ICP-ES, Varian 715) (Figure S5).

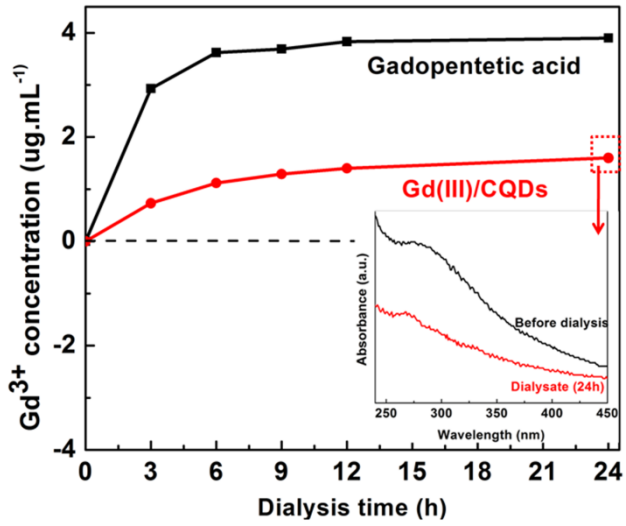

Figure S5 The concentration of Gd^{3+} ions passing into dialysate at different time during dialysis of gadopentetic acid and Gd(III)/CQDs, respectively. Inset: the UV-vis spetra of dialysate (after dialysis of Gd(III)/CQDs for 24h) and the Gd(III)/CQDs before dialysis.

6. Photoluminescence properties of Gd(III)/CQDs

Table S1 The maximum emission wavelength (λ_{em}), maximum excitation wavelength (λ_{ex}), Stokes shift and FWHM of Gd(III)/CQDs prepared at different temperatures.

Pyrolysis temperature (°C)	λ_{em}/nm	λ_{ex}/nm	Stokes shift/nm	FWHM/nm
250	436	360	86	102
300	442	375	92	134
350	434	368	84	110

7. Dispersibility of Gd(III)/CQDs

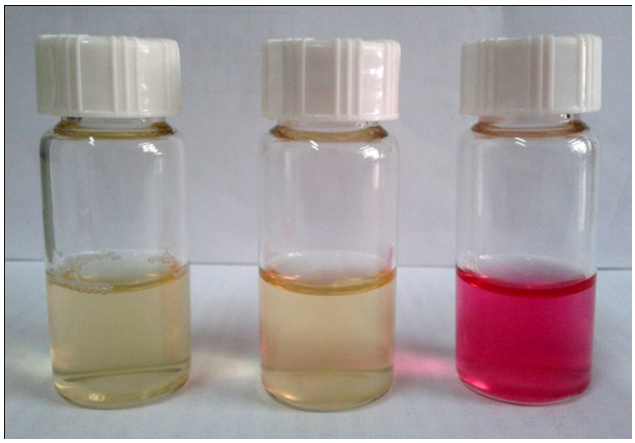

Figure S6 Gd(Ⅲ)/CQDs solution in water, phosphate-buffered saline buffer solution and culture medium with a concentration of 2 $mg \cdot mL^{-1}$