## **Electronic Supplementary Information**

## Carbon quantum dots with intrinsic mitochondrial targeting ability for

## mitochondria-based theranostics

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Xian-Wu Hua and Yan-Wen Bao have contributed equally to this paper.

**Table S1** The QYs of six types of CD samples synthesized with different proportions of the three components: chitosan (denoted as "a"), ethylenediamine (denoted as "b") and mercaptosuccinic acid (denoted as "c").

CDs: a (1 g) + b + c						
b (μL)	50	100	200	500	500	500
c (mg)	500	500	500	500	250	1000
QY (%)	8.7	8.3	11.8	7.5	9.7	6.4

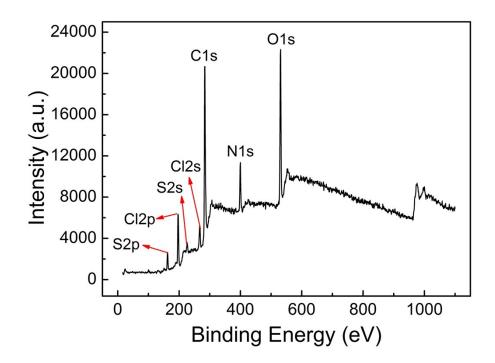
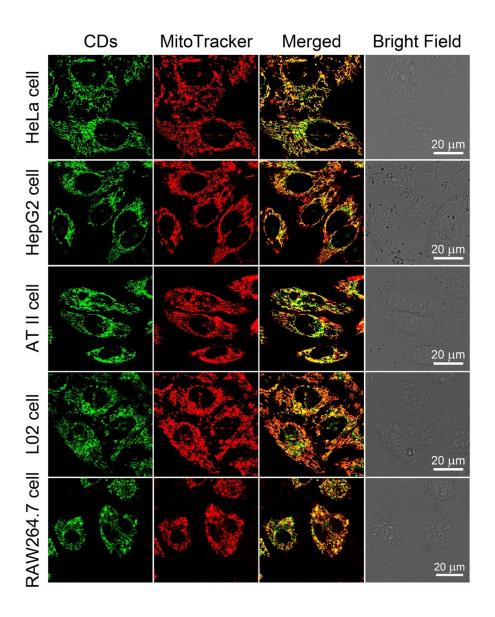


Fig. S1 XPS spectrum of dried CDs.



**Fig. S2** Mitochondrial localization of CDs in different cells including HeLa, HepG2, AT II, L02 and RAW264.7. Cells were incubated with CDs for 30 min and then co-stained by MitoTracker for another 30 min.

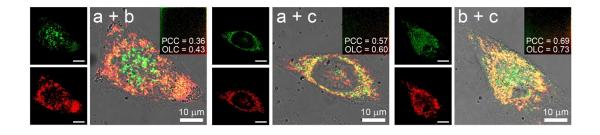
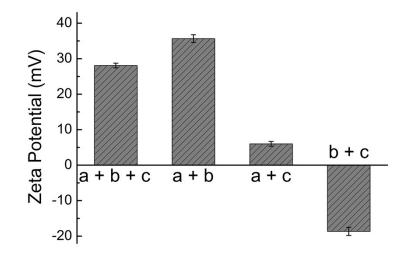
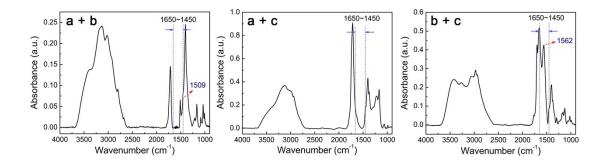


Fig. S3 Confocal images of MCF-7 cells co-stained by the control CDs (Ex = 488 nm)

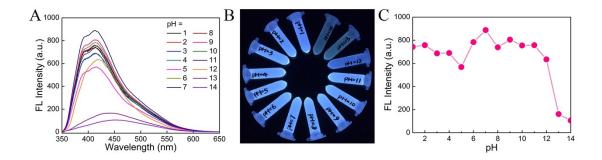
and MitoTracker (Ex = 638 nm), respectively. The three types of control CDs (a + b, a + c and b + c) were synthesized by two of the three components: chitosan (a), ethylenediamine (b) and mercaptosuccinic acid (c). Inset: The intensity correlation plots of CDs with MitoTracker.



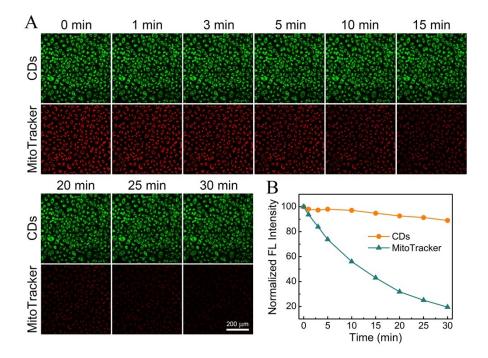
**Fig. S4** Zeta potential values of the four types of CDs prepared by hydrothermal treatment of different combinations of the three raw materials as indicated.



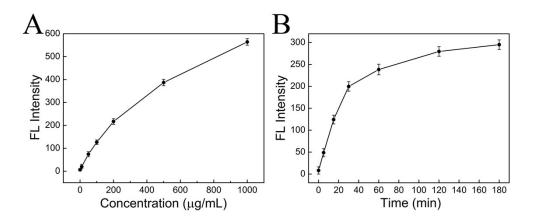
**Fig. S5** FTIR spectra of the three control CDs prepared by hydrothermal treatment of different combinations of the three raw materials as indicated.



**Fig. S6** (A) Fluorescence spectra (*Ex*: 327 nm) and (B) photographs taken under a 365 nm UV lamp of CDs dissolved in aqueous solutions with different pH values (1–14). (C) The corresponding change of the FL intensity (at 418 nm) of CDs with the solution pH.



**Fig. S7** (A) Confocal fluorescence images of CDs/MitoTrakcer-stained MCF-7 cells after continuous irradiation for different time periods. (B) Photostability comparison of CDs and MitoTracker. Fluorescence intensities were collected from the confocal images of MCF-7 cells stained with CDs and MitoTracker, respectively.



**Fig. S8** The fluorescence intensities of MCF-7 cells incubated with (A) CDs of different concentrations (0–1000  $\mu$ g/mL) for 30 min and (B) 100  $\mu$ g/mL of CDs for different time periods (0–180 min).

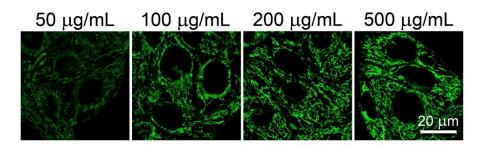


Fig. S9 Confocal fluorescence images of MCF-7 cells stained with CDs of different concentrations (50, 100, 200 and 500  $\mu$ g/mL) for 30 min.

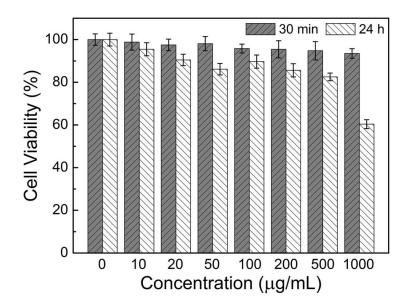
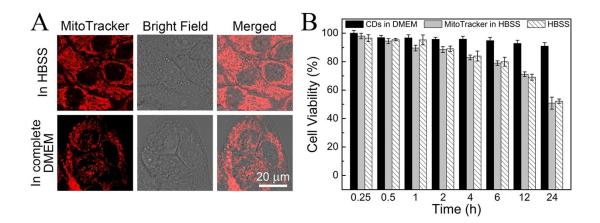
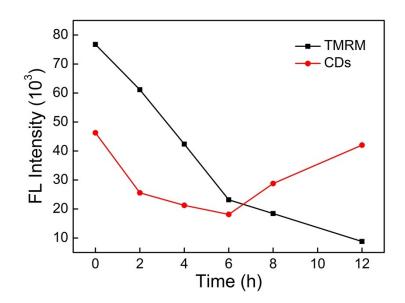


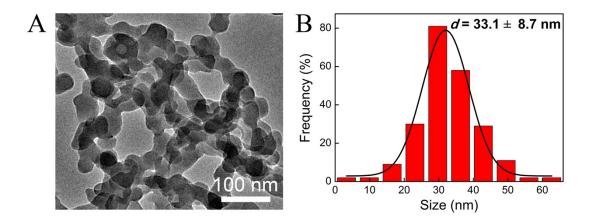
Fig. S10 Viabilities of MCF-7 cells after treatment with CDs of different concentrations (0–1000  $\mu$ g/mL) for 30 min or 24 h.



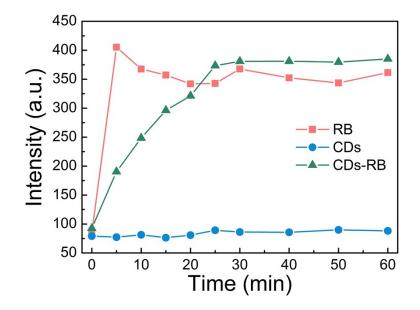
**Fig. S11** (A) Confocal images of MCF-7 cells stained by MitoTracker ( $0.5 \mu$ M) for 30 min in HBSS or in complete DMEM. It can be seen that MitoTracker did not work well in complete DMEM. (B) Cytotoxicity of CDs (100 µg/mL, in complete DMEM), MitoTracker ( $0.5 \mu$ M, in HBSS) and HBSS to MCF-7 cells (for different incubation time periods: 15 min, 0.5, 1, 2, 4, 6, 12 and 24 h) tested by MTT assay.



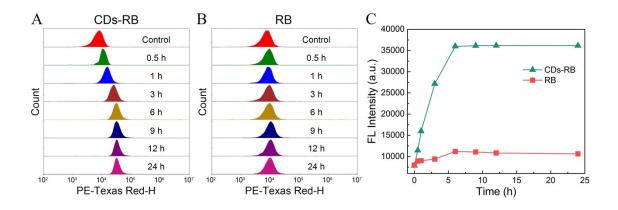
**Fig. S12** The changes of FL intensity of TMRM and CDs (in MCF-7 cells) as a function of time after the STS treatment.



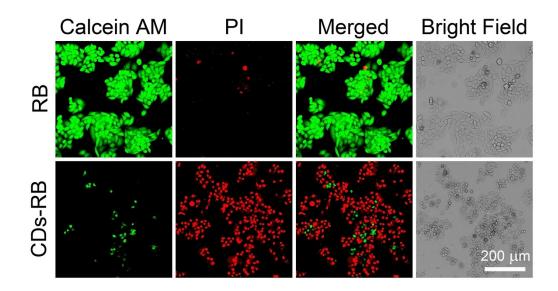
**Fig. S13** (A) TEM image and (B) the corresponding size distribution histogram of CDs-RB.



**Fig. S14** Change of the singlet oxygen sensor green (SOSG) fluorescence intensity at 526 nm of various samples (5  $\mu$ g/mL RB, 20  $\mu$ g/mL CDs and CDs-RB (RB concentration: 5  $\mu$ g/mL)) during the 532 nm laser irradiation (20 mW).



**Fig. S15** Flow cytometric analysis of MCF-7 cells incubated with CDs-RB (A) and RB (B) at different time intervals. (C) The corresponding change of the fluorescence intensities from CDs-RB and RB with time.



**Fig. S16** Live/dead staining results (using calcein-AM and PI) of MCF-7 cells after incubation with free RB or CDs-RB (5  $\mu$ g/mL of RB) for 30 min, washing with cell PBS twice, and then irradiation with a 532 nm laser (30 mW) for 5 min.