Supporting Information

Rapid and highly sensitive visual detection of oxalate for metabolic assessment of urolithiasis via selective recognition reaction of CdTe quantum dots

Piaopiao Chen,[a,#] Yunjin Bai,[a,b,#] Yin Tang,[b] Shixin Yan,[a] Xinyi Wang,[a] Wuran Wei,[b] Jia Wang,[b] Ming Zhang,[a] Binwu Ying,[a,*] and Jia Geng[a,*]

[a] *Department of Laboratory Medicine, State Key Laboratory of Biotherapy and Cancer Center, West China Hospital, Sichuan University and Collaborative Innovation Center for Biotherapy, Chengdu, Sichuan, 610041, China*

[b] *Department of Urology, Institute of Urology, West China Hospital, Sichuan University, Chengdu, Sichuan, 610041, China*

**Corresponding authors. E-mails: geng.jia@scu.edu.cn; yingbinwu@scu.edu.cn.*

[#]*Piaopiao Chen and Yunjin Bai contributed equally to this work.*

Reagents. All reagents used in this work were of analytical-reagent or higher grade and used without further purification. High purity $NaNO_3$, $Mg(NO_3)_2$, NaOH, NaCl, KCl, cadmium chloride ($CdCl_2 \cdot 2.5H_2O$), sodium tellurite (Na_2TeO_3), NaH_2PO_4, Na_2HPO_4, $CaCl_2$, $MgCl_2$, and potassium borohydride (KBH_4) were purchased from Kelong Chemical Reagents (Chengdu, China). CuCl and $CuCl_2$ were obtained from Shanghai Sangon Biotechnology Co., Ltd (Shanghai, China). 3-(N-Morpholino) propanesulfonic acid (MOPS) was purchased from Solarbio Technology Co., Ltd (Beijing, China). Glucose, urea, and oxalate were purchased from Sigma Company (Shanghai, China). $CuSO_4$, and 3-mercaptopropionic acid (MPA) was obtained from Aladdin Reagent Co. Ltd (Shanghai, China). Human urine samples were donated from the West China Hospital of Sichuan University (Chengdu, China). All work solutions were prepared with 10 mM pH 7.4 MOPS buffer (100 mM $NaNO_3$, 2.5 mM Mg $(NO_3)_2$). High purity deionized water (18.2 MΩ-cm) was obtained from Milli-Q water system (Chengdu Ultrapure Technology Co., Ltd., Chengdu, China). All solutions were stored at 4 °C in a refrigerator until use.

Instruments. The absorption spectrum of CdTe QDs was recorded by a Hitachi U-1750 UV-vis spectrophotometer (Shimadzu, Kyoto, Japan). High-resolution transmission electron microscope (HR-TEM) measurements of CdTe QDs were carried out by a Tecnai G2F20 STWIN TEM at an accelerating voltage of 200 kV (FEI Co., USA). The energy disperse spectroscopy (EDS) images of CdTe QDs measurements were carried out with a field emission scanning electron microscope (SEM, JSM-7800F, JEOL, Japan). An X-ray diffractometer (X'Pert Pro MPD, Philips, Netherlands) using Cu Kα radiation was used to

record the powder X ray diffraction (PXRD) patterns. The survey scan and Hg images of the CdTe QDs were carried out on a K-Alpha 1063 X-ray photoelectron spectroscopy (XPS, Thermo Fisher Scientific, England). An F-7100 spectrometer (Hitachi, Japan) and the Duetta Spectrophotometer (HORIBA Canada Inc) were used to record the fluorescence signal of CdTe QDs. The buffers' pH was determined by PHS-3C pH Benchtop meter (INESA, Shanghai, China). Fourier transform infrared spectra (FTIR) of CdTe QDs were collected using a Nicolet IS10 FTIR spectrometer (Thermo Inc., America). Liquid chromatography coupled with TSQ Quantum Ultra Mass Spectrometer (LC-MS) was used to detect oxalate in urine samples (Thermo Fisher Scientific, Waltham, MA, USA).

Synthesis of CdTe QDs. A one-pot synthetic method was used to prepare QDs.[1, 2] First, containing $CdCl_2$ (0.5 mmol) and trisodium citrate (0.2 g) was dissolved in 50 mL solution, followed by adding 52 μL MPA in the above solution. Then, the solution pH was adjusted to 10.5 by NaOH (0.1 M). Next, Na_2TeO_3 (0.1 mmol) and KBH_4 (50 mg) were added into the above solution, and then refluxed for 1 h to obtain the CdTe QDs solution. Finally, CdTe QDs was purified via precipitation with n-propanol and centrifugation (11 000 rpm). The purified red CdTe QDs were redispersed in high purity water before to use, and kept at 4 °C. We calculated the concentration of synthesized QDs to be 12 μM by referring to existing literature.[3]

Cell culture and cell counting kit (CCK-8) assay experiments. The human kidney cell (HK-2) and human urothelial cell (HUC) were cultured at 37 °C, 5% CO_2 in

high-glucose Dulbecco's Modified Eagle Medium (Gibco; ThermoFisher Scientific) or Kaighn's Modification of Ham's F-12 Medium (Hyclone, USA) supplemented with 10% fetal bovine serum (Gibco; ThermoFisher Scientific), 100 units/mL penicillin, and 100 μg/mL streptomycin (Gibco).

Cell viability was measured by CCK-8 assay. HK-2 and HUC cells were plated into the 96-well plate for overnight followed by treatment with CdTe QDs in different concentrations for 24 h. 10 μL CCK-8 was added into the medium (100 μL per well) and the cells were subsequently incubated at 37 °C for 2 h. For each condition, three replicates were performed. The absorbance was detected using a microplate reader at 450 nm.

References

1. P. P. Chen, X. Jiang, K. Huang, P. Y. Hu, X. Q. Li, L. Wei, W. Z. Liu, L. W. Wei, C. M. Tao, B. W. Ying, X. W. Wei and J. Geng, *ACS Appl. Mater. Interfaces*, 2019, **11**, 36476-36484.
2. P. Y. Hu, X. Wang, L. Wei, R. Dai, X. Yuan, K. Huang and P. P. Chen, *J. Mater. Chem. B*, 2019, **7**, 4778-4783.
3. W. W. Yu, L. H. Qu, W. Z. Guo and X. G. Peng, *Chem. Mater.*, 2003, **15**, 2854-2860.