

## Electronic Supplementary Information

### **Cyclodextrin-clicked Silica/CdTe Fluorescent Nanoparticles for Enantioselective Recognition of Amino Acids**

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#### **1. Materials and instruments**

Tellurium (Te), cadmium chloride hydrate ( $\text{CdCl}_2 \cdot 2.5\text{H}_2\text{O}$ ), 3-mercaptopropionic acid (3-MPA) were obtained from Aladdin (Shanghai, China). Amino acids, tetraethylorthosilicate (TEOS), (3-Mercaptopropyl)trimethoxysilane (KH-590), sodium borohydride ( $\text{NaBH}_4$ ), thiourea, sodium azide and  $\beta$ -CD were purchased from Energy Chemical Co., Ltd. (Shanghai, China). All reagents were of analytical grade and used directly without further purification.

Fourier-transform infrared spectra were recorded on Thermo Scientific Nicolet iS-10 FT-IR (Thermo Fisher Scientific, USA). The absorption spectra were obtained from an Evolution 220 UV-vis instrument (Thermo Fisher Scientific, USA). The photoluminescence experiments were performed on a RF-5301 luminescence spectrometer (Shimadzu, Japan). Structural and compositional investigations of as-prepared QDs were conducted on a FEI Tecnai G2 F30 transmission electron microscope (FEI, USA).

#### **2. Preparation of CD/SiO<sub>2</sub>/CdTe QDs**

##### **2.1 Preparation of 3-MPA stabilized CdTe QDs<sup>[1-2]</sup>**

Te (38.3 mg, 0.3 mmol) and excess  $\text{NaBH}_4$  (22.7 mg, 0.6 mmol) was mixed in

oxygen-free deionized water (10 mL) with an ice-bath at nitrogen atmosphere. The reaction was kept for 4 h and an achromatic NaHTe solution was obtained. CdCl<sub>2</sub>•2.5H<sub>2</sub>O solution (68.5 mg, 0.3 mmol in 100 mL of deionized water) was pretreated with 26 μL of 3-mercaptopropionic acid (26 μL, 0.3 mmol) with vigorous stirring for 20 min and the pH was adjusted to 10.0 using 0.1 M NaOH solution. Then, the as-prepared NaHTe solution (2 mL) was injected to the mixture with stirring for 10 min to form 3-MPA stabilized CdTe precursors. The mixture was heated to 90 °C and refluxed under the nitrogen atmosphere for 3 h. The resulted CdTe QDs was collected and stored at 4 °C for further use.

## ***2.2 Preparation of SiO<sub>2</sub>/CdTe QDs***

The CdTe QDs solution (20 mL) was added into ethanol (10 mL) with stirring for 20 min, followed by the addition of different amount of KH-590 (2, 4, 6, 10, 20 μL). The mixture was kept stirring for 20 min and then the volume was adjusted to 50 mL at pH=9. The CdTe QDs were thus encapsulated within SiO<sub>2</sub> nanoparticles via hydrolysis/condensation of KH-590 in the mixed solvents of water and ethanol. The as-prepared SiO<sub>2</sub>/CdTe QDs was stored at refrigerator.

## ***2.3 Clicked preparation of silanized 6-azido-β-CD***

### ***2.3.1 Synthesis of N-(3-triethoxysilanepropyl)-2-propiolamide***

Under the protection of nitrogen, 3-aminopropyltriethoxysilane (4.8 g, 21.7 mmol) was dissolved in dry CH<sub>2</sub>Cl<sub>2</sub> (30 mL). Then, propiolic acid (1.74 g, 24.8 mmol) and N,N'-dicyclohexylcarbodiimide (4.92 g, 23.8 mmol) was added successively, the mixture was kept stirring for 2.5 h. The solvent was removed after filtration to obtain crude product. Afterwards, dry toluene was added and rotary evaporated to remove the solvent (three times) affording yellow oily N-(3-triethoxysilanepropyl)-2-propiolamide (4.8 g, 81%).

### ***2.3.2 Clicked preparation of silanized β-CD<sup>[3-4]</sup>***

N<sub>3</sub>-CD (2 g, 1.72 mmol), N-(3-triethoxysilanepropyl)-2-propiolamide (0.47 g, 1.72 mmol) and CuI(PPh<sub>3</sub>) (77.9 mg, 0.172 mmol) was dissolved in dry DMF (40 mL).

The click reaction was conducted for 2 d at 90 °C. The resulted mixture was added to acetone (100 mL) to precipitate pale yellow product, which was re-dissolved in DMF (10 mL) and tetraethoxysilane (2 mL) was added with ultrasonic treatment. The supernatant after centrifugation was obtained and stored for further use. The  $^1\text{H}$  NMR spectra (500 MHz,  $\text{DMSO-d}_6$ ) of target product was depicted in Fig.S1. The peak at 8.13 ppm was assigned to (CH=C) and the peaks between 1.5-1.0 ppm were assigned to the protons of  $-(\text{CH}_2)_3\text{Si}(\text{OEt})_3$ .

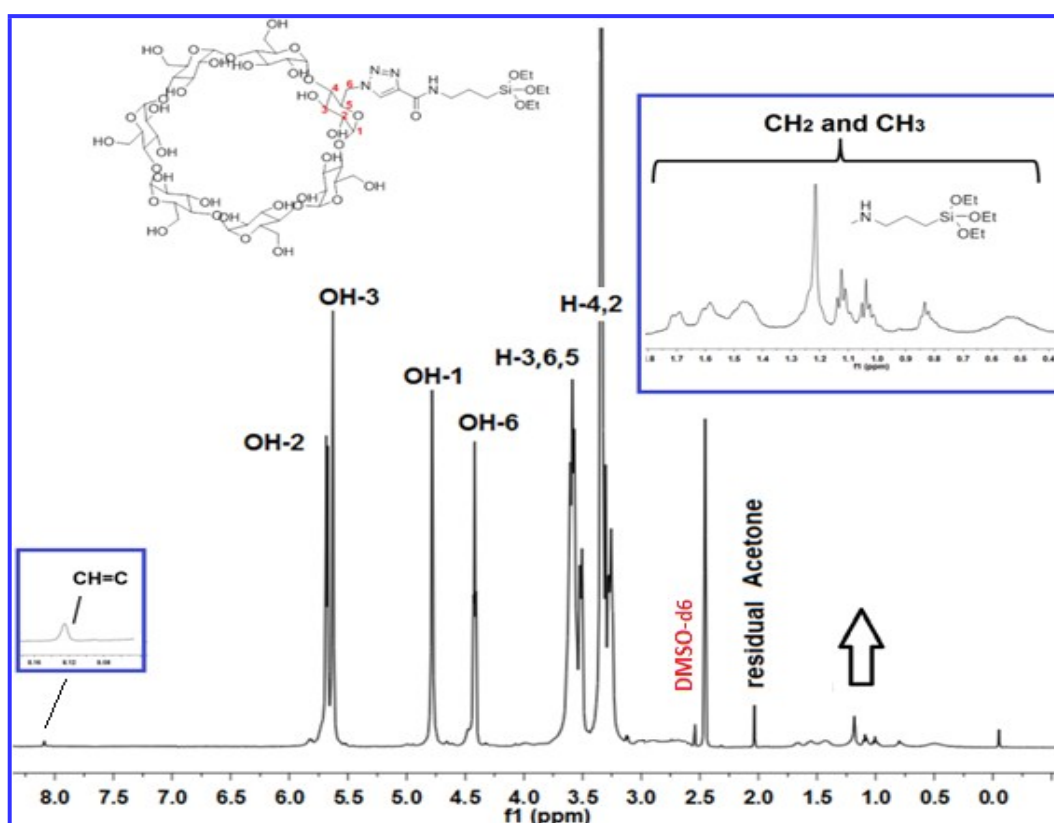


Fig. S1  $^1\text{H}$  NMR spectra of silanized  $\beta$ -CD.

#### 2.4 Preparation of CD/SiO<sub>2</sub>/CdTe NPs

The silanized CD solution was added into as-prepared SiO<sub>2</sub>/CdTe NPs solution with vigorous stirring for 30 min varying the CD solution from 100  $\mu\text{L}$  to 3mL. The crude product was washed with ethanol for three times and dried under vacuum and then dissolved in buffer for the chiral recognition of amino acids. All the samples were diluted three-folds using buffer prior to use.

### 3. Optimization of the preparation of CD/SiO<sub>2</sub>/CdTe NPs

By varying the addition volume of KH-590 from 2 to 20  $\mu\text{L}$ , the PL intensity dramatically declined when the amount exceeded 6  $\mu\text{L}$  (Fig.S2a). Adequate KH-590 can lead to improved size of silica nanoparticles advantageous for the further anchoring of CD, while too low concentration would insufficient encapsulation leading to QDs bare in solution. Considering the PL intensity and further modification, 6  $\mu\text{L}$  was selected to form first silica layer on the surface of CdTe QDs. Similarly, decreased PL intensity was observed with more CD amount (Fig. S2b). As a compromise, the CD amount was moderated as 500  $\mu\text{L}$  to guarantee sufficient host cavity to capture guest molecules. The CD/SiO<sub>2</sub>/CdTe NPs were prepared following as-optimized condition for further chiral recognition of amino acids.

### 4. References

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