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Electronic Supporting Information for

Surface characterization of thiol ligands on CdTe quantum dots: analysis by ^{1}H NMR and DOSY

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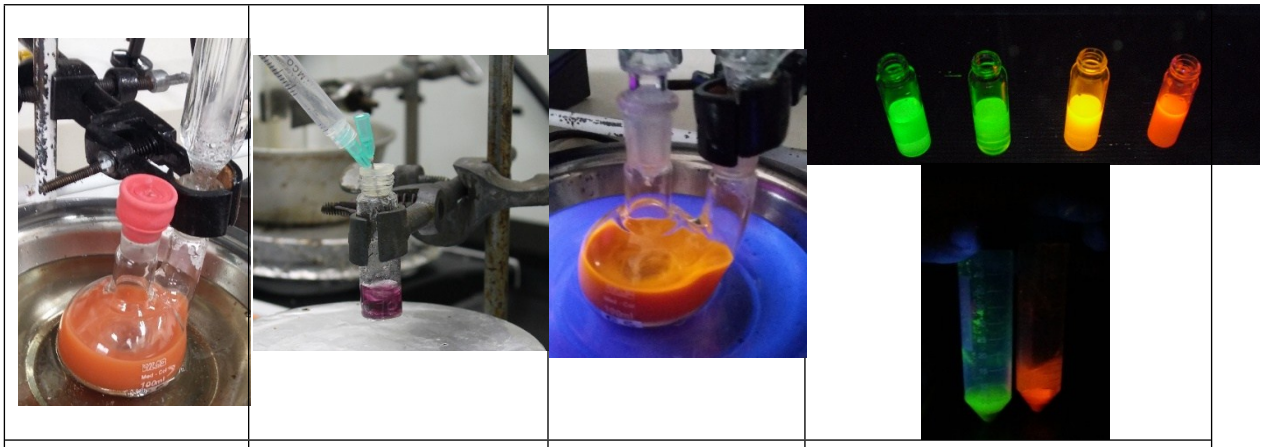
Table of Contents

		Pages
1	**Synthetic procedure**	S2
2	**NMR experiments**	S2

1. Synthetic procedure

CdTe QDs were synthesized by mixing 4 mmol of $CdCl_2$, 3.2 mmol of tioglicolic acid (TGA), and 200 mL of deionized water (DI) in a 250 mL three-neck flask under vigorous stirring and argon inert atmosphere. A 2.0 N NaOH solution was slowly added to adjust the pH of the mixture to 10. The chalcogenide precursor was prepared mixing 0.6 mmol $NaBH_4$ and 0.2 mmol Te in 5 mL of DI water under vigorous stirring under inert atmosphere. The freshly prepared NaHTe solution was quickly injected into the Cd-thiol ligand precursor solution and the final mixture was refluxed for 0.5, 1, 4 and 10 h. The obtained CdTe-TGA QDs were purified by centrifugation at 5000 rpm for 15 min, followed by successive dissolution and precipitations sequential process using acetone and DI water.



Reaction setup	Preparation of NaHTe	Reaction setup under UV (235 nm)	Precipitated CdTe-TGA QDs (0.5 and 4 h)

Fig. 1S. Visual steps of procedure for CdTe-TGA preparation.

2. NMR experiments

The NMR measurements were obtained with a Bruker Advance-III spectrometer operating at 400.16 MHz. Samples were prepared dissolving 3 mg of each QDs in 450 µL of D_2O (Merck, 99.8 % D) or DMSO (Merck, 99.8 % D). ^{1}H-DOSY experiments were carried out by a pulse field gradient spin-echo PFGSE decay (pulse sequence *ledbpgp2s* by Bruker). A diffusion time (big delta) of 0.05 s and P30 (1300 µs) were used; the diffusion coefficient

(DC) values and the viscosity (η) of 1.0963 mPa s for D_2O were used to calculate the hydrodynamic radius (dH) according to the Stokes-Einstein equation. All experiments were performed at 298 K and Topspin 2.1 software was used for processing all spectra. With the experimental parameters optimized, full signal attenuation was achieved after 32 steps of linearly increasing the gradient strength from 2% to 95%. About 3 mg of each sample were dissolved in 450 µL of D_2O.

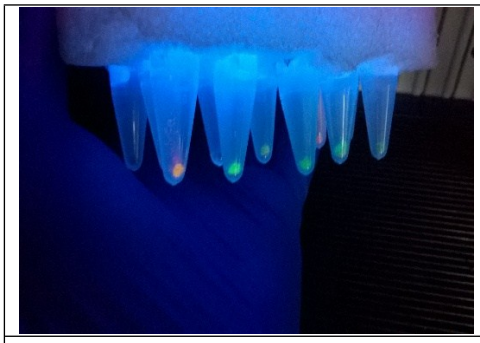
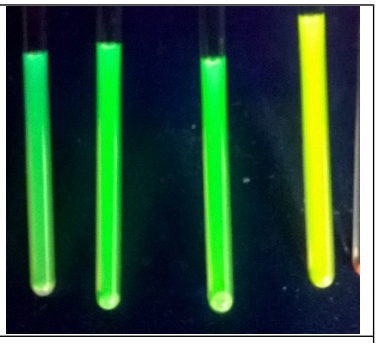
		
QDs Samples (□ 3 mg)	Sample dissolved in D_2O 99.9% (NMR tube)	Selected samples analysed by NMR (0.5 h and 1 h)

Fig. 2S. Visual steps of NMR experiments.