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

<table>
<thead>
<tr>
<th></th>
<th>Pages</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Synthetic procedure</td>
</tr>
<tr>
<td>2</td>
<td>NMR experiments</td>
</tr>
</tbody>
</table>
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.

![Image](image.jpg)

**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$_2$O (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 ($\eta$) of 1.0963 mPa s for D$_2$O 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$_2$O.

**Fig. 2S.** Visual steps of NMR experiments.