

*Supplementary Materials*

# Detecting CdSe Nanomaterials with a Fluorescent Schiff Base Ligand

Jesús Sanmartín-Matalobos <sup>1,\*</sup>, Pilar Bermejo-Barrera <sup>2</sup>, Ignacio Pérez-Juste <sup>3</sup>, Matilde Fondo <sup>1</sup>, Ana M. García-Deibe <sup>1,\*</sup> and Yeneva Alves-Iglesias <sup>1,2</sup>

<sup>1</sup> Coordination and Supramolecular Chemistry Group (SupraMetal), Department of Inorganic Chemistry, Faculty of Chemistry, Institute of Materials (iMATUS), Universidade de Santiago de Compostela, Avenida das Ciencias s/n, 15782 Santiago de Compostela,

<sup>2</sup> Trace Element, Speciation and Spectroscopy Group (GETEE), Department of Analytical Chemistry, Nutrition and Bromatology, Faculty of Chemistry, Institute of Materials (iMATUS), Universidade de Santiago de Compostela, Avenida das Ciencias s/n, 15782 Santiago de Compostela, Spain

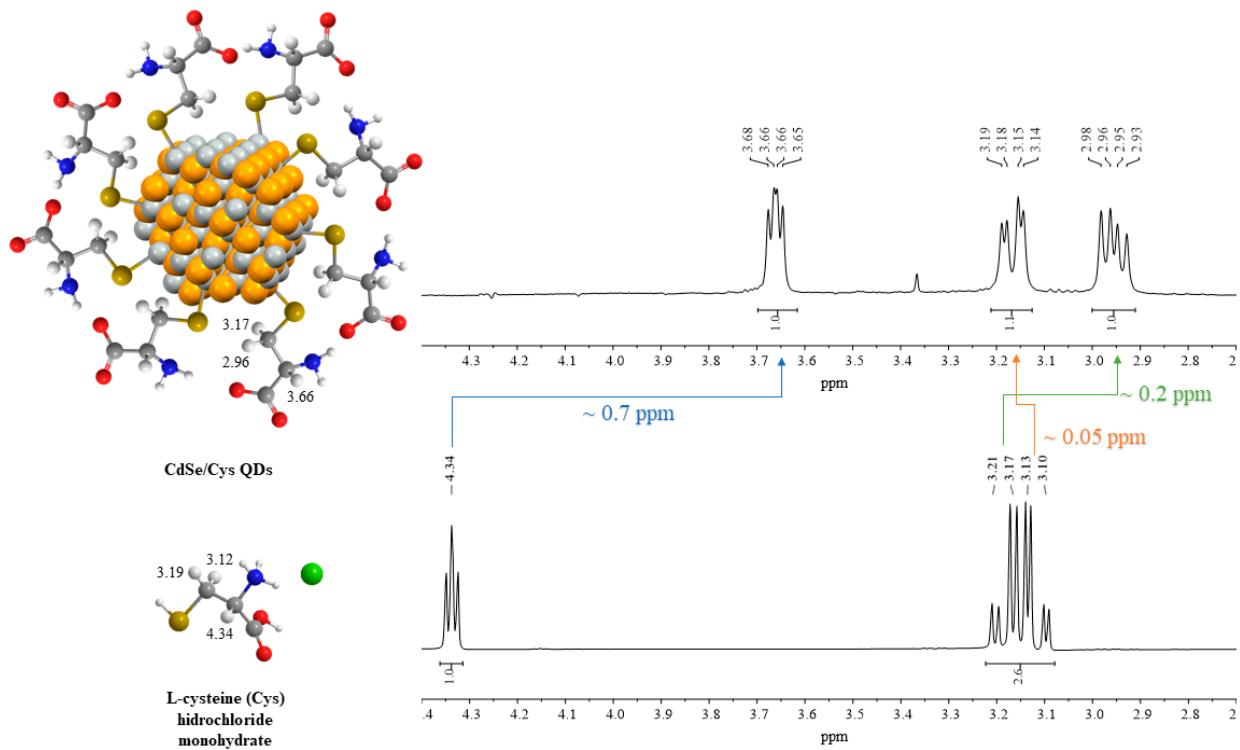
<sup>3</sup> Departamento de Química Física, Facultad de Química, Edificio de Ciencias Experimentales, Universidade de Vigo, 36310 Vigo, Spain

\* Correspondence: jesus.sanmartin@usc.es (J.S.-M.); ana.garcia.deibe@usc.es (A.M.G.-D.)

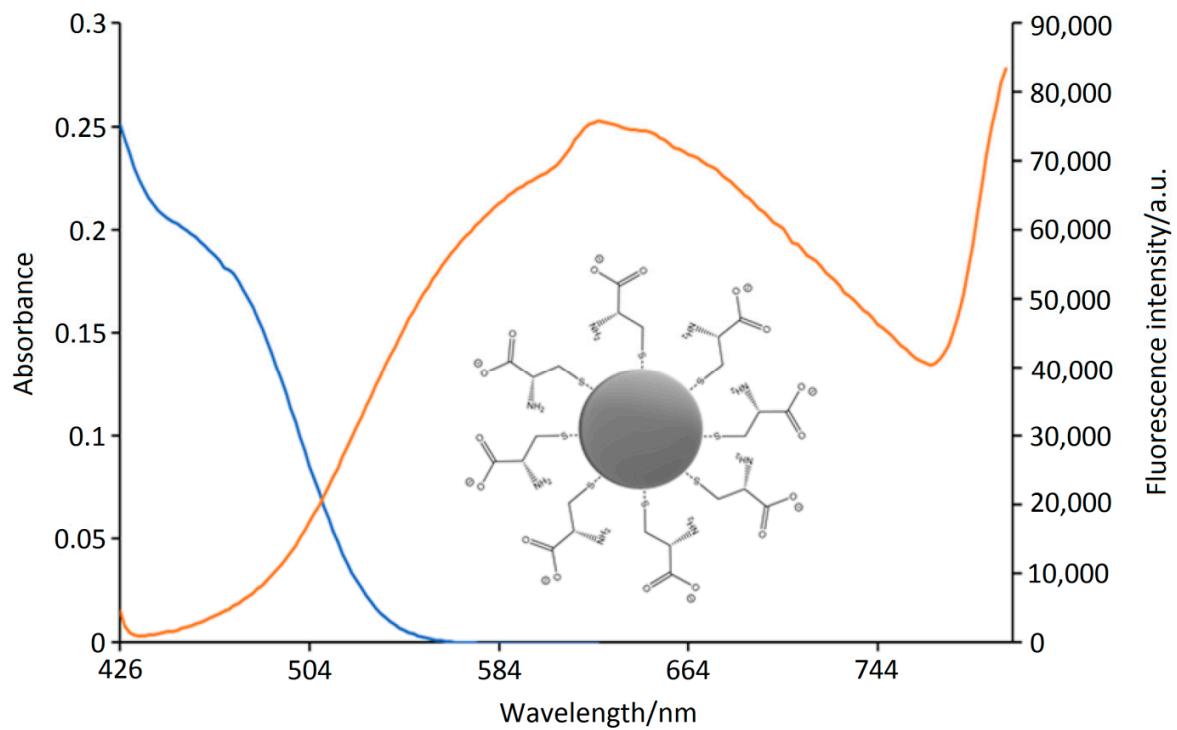
---

**Table of Contents .....** .....page

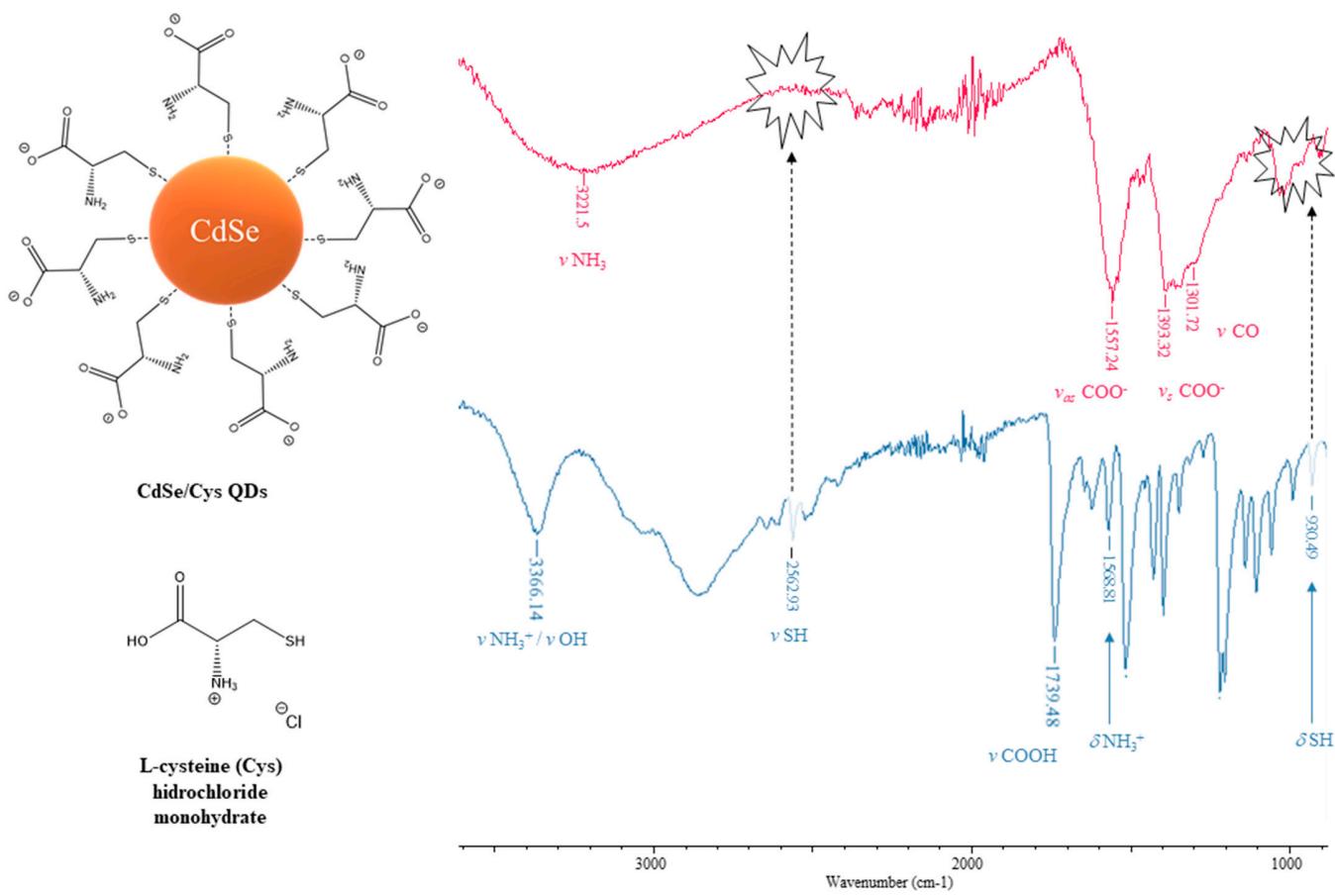
1.	<sup>1</sup> H NMR spectrum of cysteine-capped CdSe QDs .....	S2
2.	UV-Vis spectrum of CdSe-Cys QDs.....	S3
3.	ATR-FTIR spectrum of CdSe-Cys QDs.....	S4
4.	SEM-EDX images of CdSe-Cys QDs .....	S5
5.	XRF spectrum and mapping of CdSe-H <sub>3</sub> L NPs .....	S6
6.	<sup>1</sup> H NMR spectrum of CdSe-Cys-H <sub>3</sub> L QDs .....	S7
7.	ATR-IR spectra of CdSe-Cys-H <sub>3</sub> L QDs .....	S8
8.	DFT models for the interaction H <sub>3</sub> L-NMs .....	S9



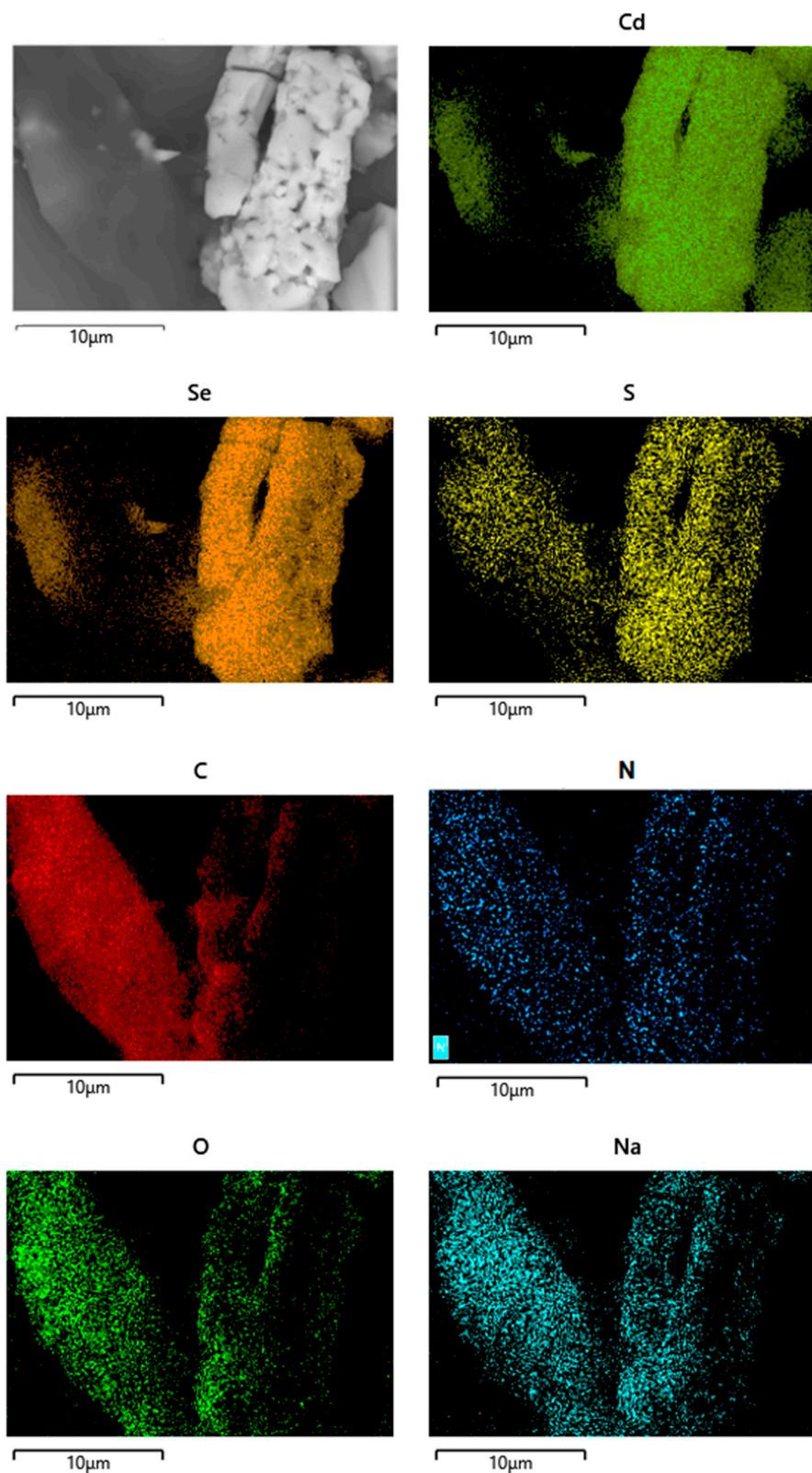
**Figure S1.** <sup>1</sup>H NMR spectrum (in D<sub>2</sub>O) of cysteine-capped CdSe QDs (**top**). The spectrum of L-cysteine (**bottom**) has been included for comparison.



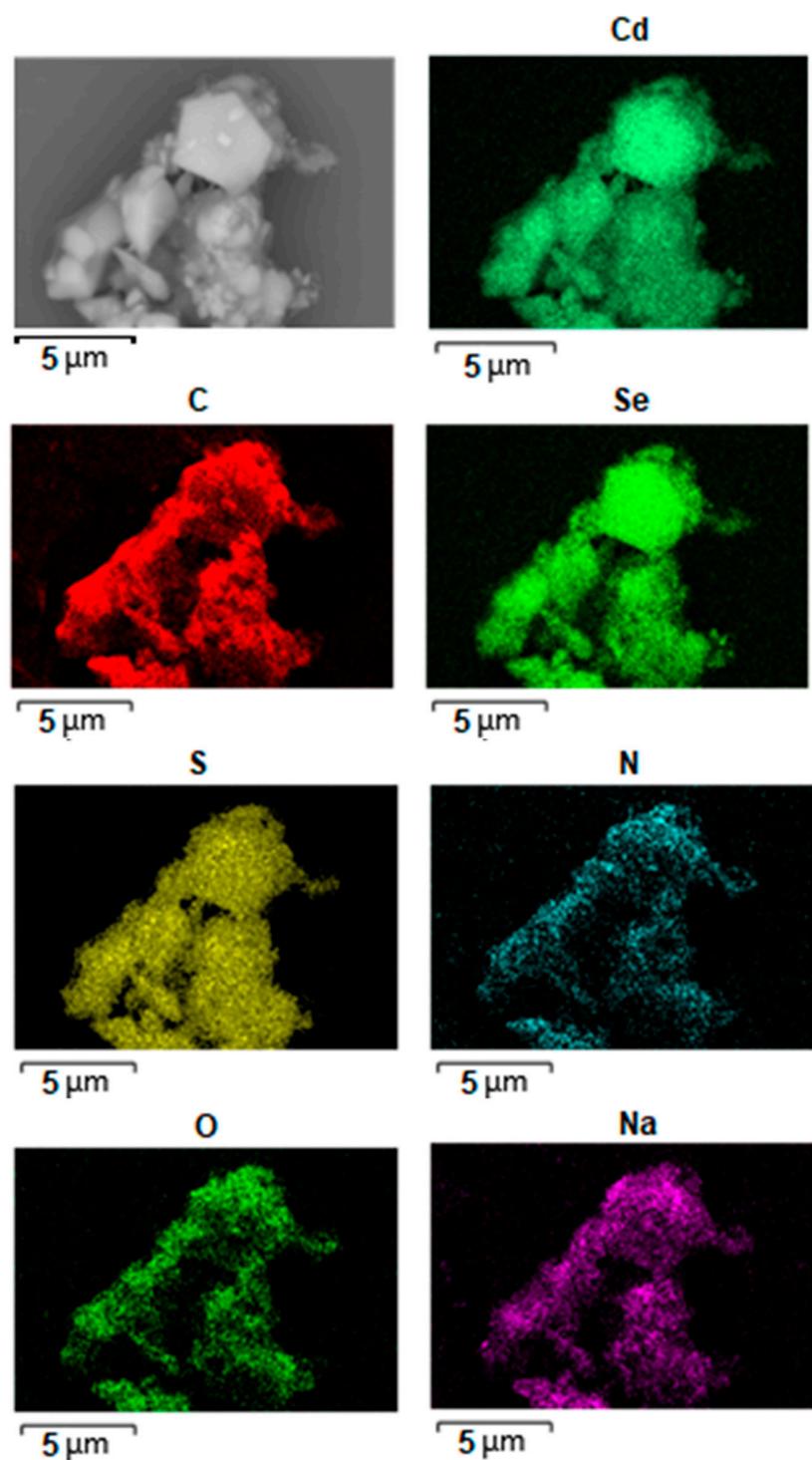
**Figure S2.** UV-Vis (**left**) and fluorescence (**right**) spectra of the cysteine-capped CdSe QDs in ethanol.



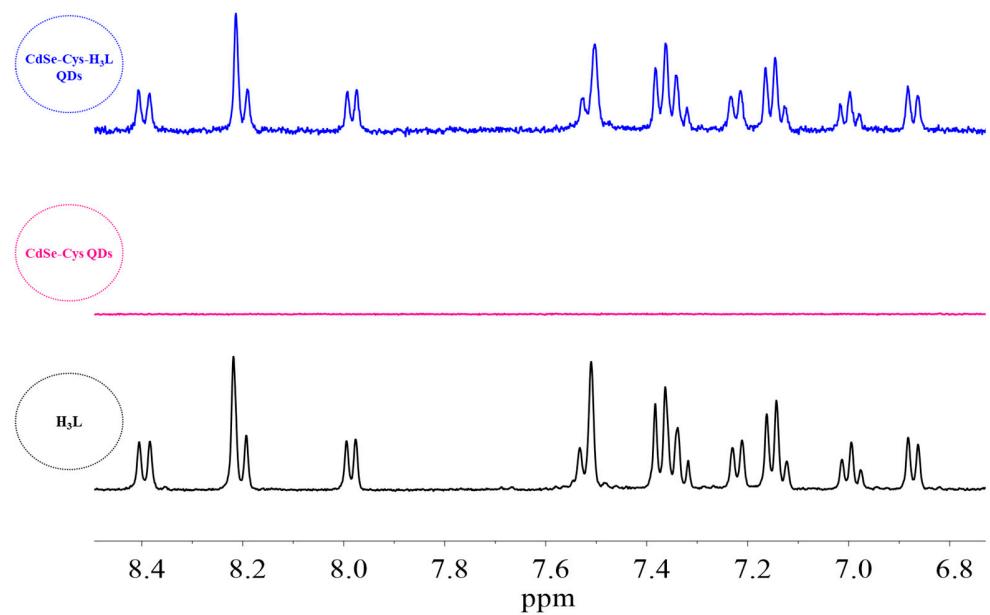
**Figure S3.** ATR-FTIR spectrum cysteine-capped CdSe QDs (**top**). The spectrum of L-cysteine (**bottom**) has been included for comparison.



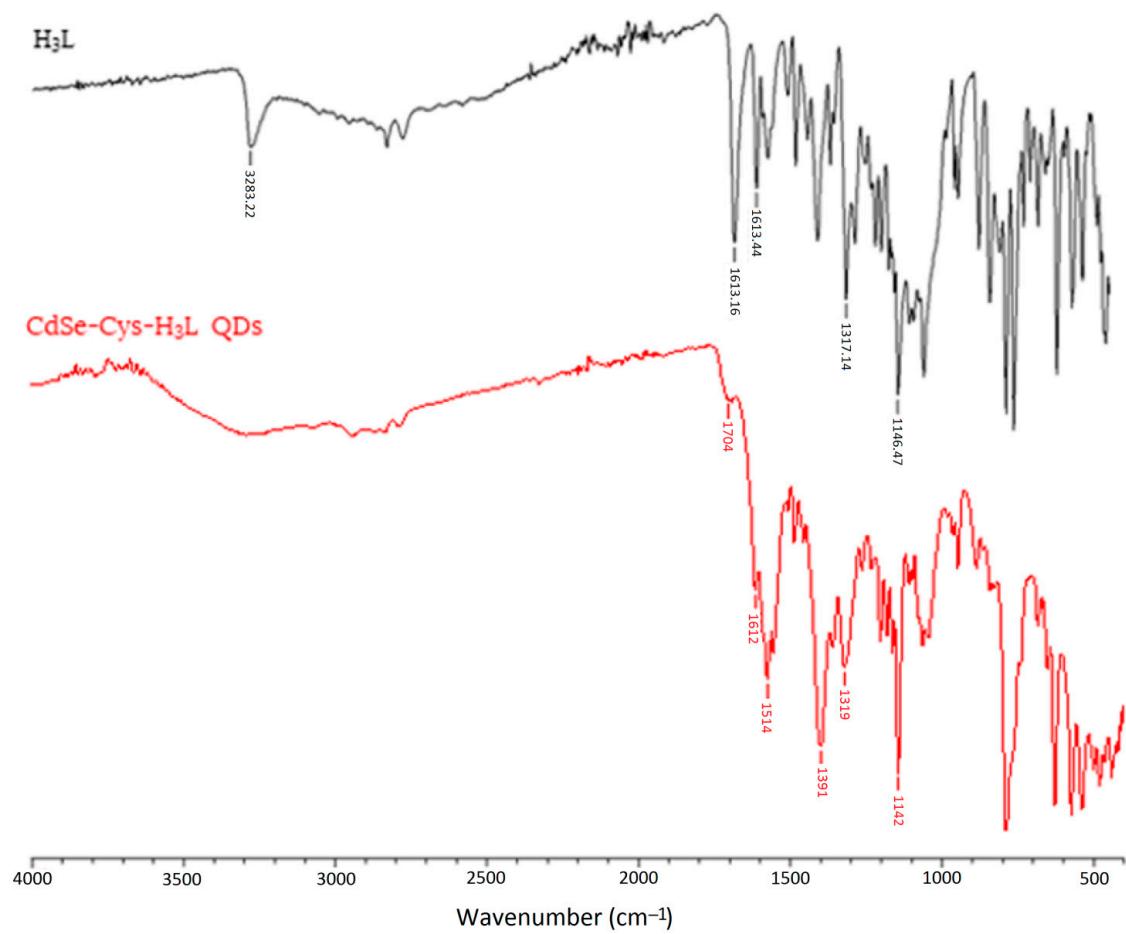
**Figure S4.** SEM micrograph of a CdSe-Cys QDs sample, and EDX mapping patterns of the elements: Cd, Se, C, S, N, Na and O. All of them have have the same spatial distribution which indicates a uniform distribution of elements.



**Figure S5.** SEM micrograph of the reaction product of CdSe-Cys QDs with H<sub>3</sub>L (as carboxylate sodium salt) and EDX mapping patterns of the elements: Cd, Se, C, N, O, S and Na .

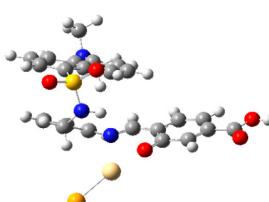
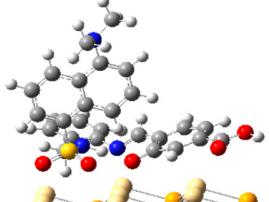
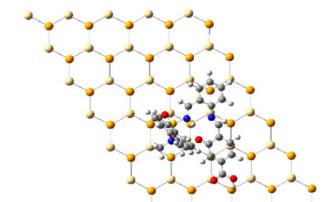
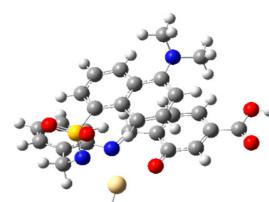
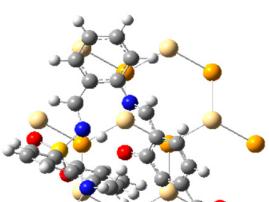
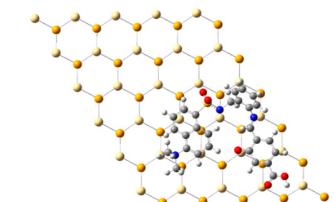


**Figure S6.** <sup>1</sup>H NMR spectra of CdSe-Cys-H<sub>3</sub>L QDs, CdSe-Cys QDs, Cys and H<sub>3</sub>L (range: 6.7 to 8.5 ppm) in methanol-d<sub>4</sub>).



**Figure S7.** ATR-IR spectra of H<sub>3</sub>L (**top**) and Cys-CdSe-H<sub>3</sub>L QDs (**bottom**).

**Table S1.** DFT models for the interaction H<sub>3</sub>L-NMs.

	1CdSe	7CdSe	35CdSe
Monoanionic			
	-70.1	-98.3	-110.2
Dianionic			
	-102.6	-155.8	-197.6