## **Supporting Information for**

## Single-step synthesis of high-quality ZnSe/ZnS quantum dots capped

## by N-acetyl-L-cysteine via hydrothermal method

Dan Zhao<sup>a</sup>, Jiao-Tian Li<sup>a</sup>, Fang Gao<sup>a</sup>, Cui-ling Zhang<sup>b</sup>, Zhi-ke He<sup>\*,b</sup> <sup>a</sup>College of Pharmacy, South-Central University for Nationalities, Wuhan 430074, PR China <sup>b</sup>Key Laboratory of Analytical Chemistry for Biology and Medicine (Ministry of Education), College of Chemistry and Molecular Sciences, Wuhan University, Wuhan 430072, P. R. China.

\*Corresponding Author: E-mail address: <u>zhkhe@whu.edu.cn</u> (Z.K.He)

Fig. S1 The QYs of NAC-capped ZnSe/ZnS QDs prepared at different reaction temperature.

Fig. S2 The effect of heating temperature on the maximum emission wavelength of NAC-capped ZnSe/ZnS QDs.

Fig. S3 The QYs of NAC-capped ZnSe/ZnS QDs prepared at different heating times.

**Fig. S4** The effect of heating time on the maximum emission wavelength of NAC-capped ZnSe/ZnS QDs.

Fig. S5 The QYs of NAC-capped ZnSe/ZnS QDs prepared at different pH values.

Fig. S6 The QYs of NAC-capped ZnSe/ZnS QDs prepared at different HSe<sup>-</sup>/Zn<sup>2+</sup> values.

Fig. S7 The QYs of NAC-capped ZnSe/ZnS QDs prepared at different NAC/Zn<sup>2+</sup> values.

**Fig. S8** PL Intensity of NAC-capped ZnSe/ZnS QDs dissolved in PBS buffer solution of different pH.



Fig. S9 XPS survey spectrum of NAC-capped ZnSe/ZnS QDs.

## Information on the calculation of the QY

The quantum yield of the sample (QYs) can be calculated using the following equation:  $QYs = (Fs \times Ar \times QYr \times N_s^2)/(Fr \times As \times N_r^2)$ 

where subscript of x and r represent sample and reference, respectively; A, N and F mean QYs, absorbance at excitation wavelength(310nm), refractive index and integral area of fluorescence, respectively. In this work, the solvent of Quinine sulfate is sulfuric acid solution (50mM), and

QDs' solvent is ultrapure water. Since QDs and quinine sulfate are both aqueous solution,  $N_s$  equates to N<sub>r</sub>. The sample and reference are both diluting solutions and the UV absorptions at 310 nm are less than 0.1. The QYs of the reference is 54.6%.

Through the calculation, the QYs of the prepared QDs synthesized under optimal condition are higher than 30%, and the best ones reach as high as 39.3%.

Table 51. The Q13 of the reference and QD3 solutions			
	A <sub>310</sub>	F ( $\lambda_{ex}$ =310nm)	QY(%)
quinine sulfate	0.0670	30664.1973	54.6
QDs	0.0708	23339.9951	39.3

Table S1. The QYs of the reference and QDs solutions