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Electronic Supplementary Information

One-step synthesis of $CuMo_2S_3$ nanocrystals for synergistic combination of photothermal therapy and photodynamic therapy

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Supplementary Figures and calculation of photothermal conversion efficiency (η)

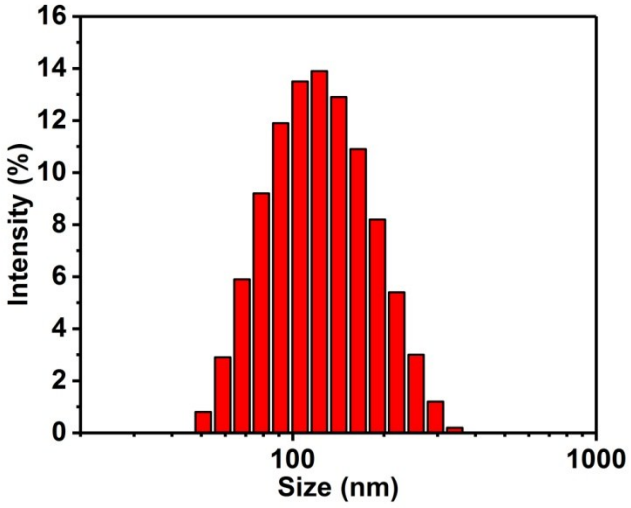

Fig. S1 Size distribution of $CuMo_2S_3$ NCs.

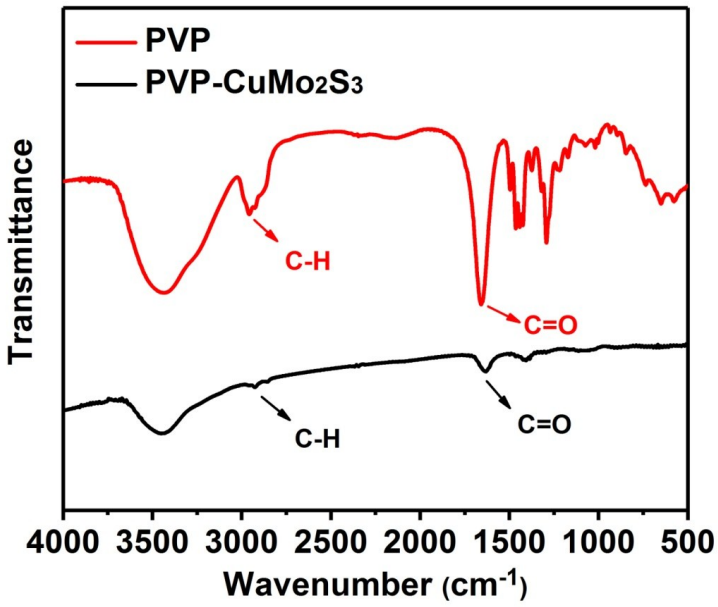

Fig. S2 Fourier transform infrared spectroscopy (FT-IR) analysis of PVP and PVP-$CuMo_2S_3$ NCs.

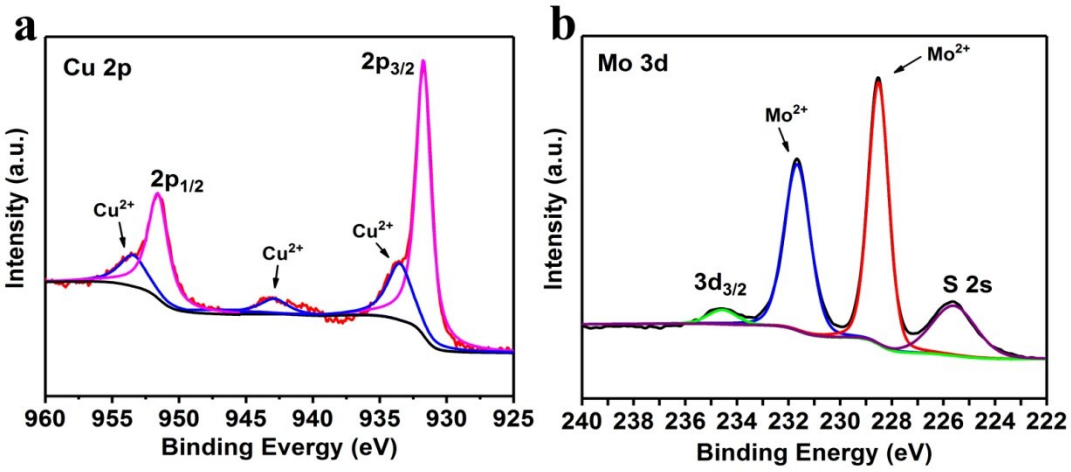

Fig. S3 XPS of (a) Cu 2p, and (b) Mo 3d.

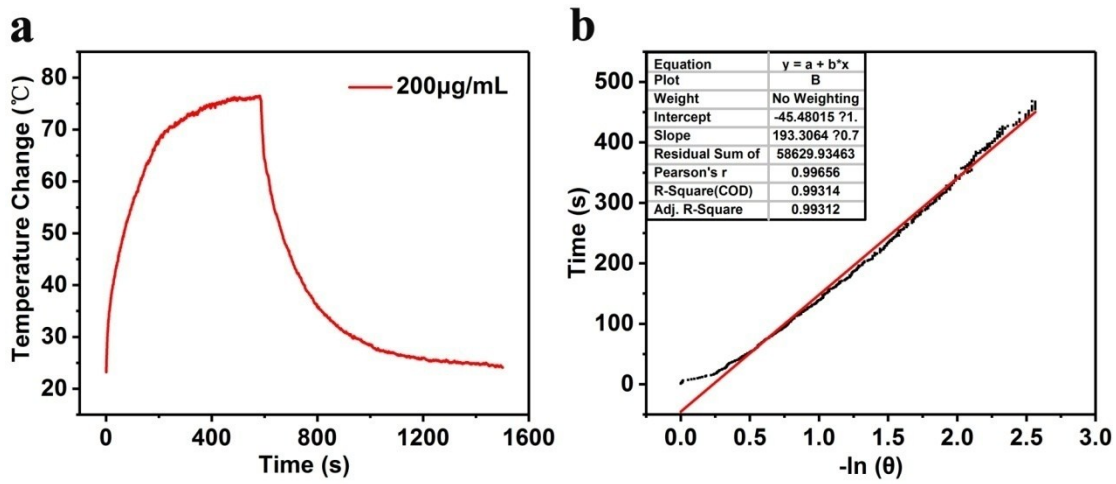

Fig. S4 (a) Temperature variations of solution containing 200 μg/mL $CuMo_2S_3$ NCs. The NIR laser irradiation lasted 600s and then was turned off. (b) Linear relation between the t and -lnθ.

Here, the photothermal conversion efficiency (η) of $CuMo_2S_3$ NCs can be calculated by previous literature,[1] $CuMo_2S_3$ NCs aqueous dispersion (200 μg mL^{-1}, 0.2 mL) was irradiated with the NIR laser (808 nm, 1.0 W cm^{-2}) until the solution reached a steady-state temperature and then the laser was turned off. The system temperature was cooled down to the ambient temperature.

$$\eta = \frac{hS(T_{max} - T_{surr}) - Q_{Dis}}{I\left(1 - 10^{-A_\lambda}\right)}$$

where h is the heat transfer coefficient, S is the surface area of sample well, T_{max} and T_{surr} are the equilibrium temperature and ambient temperature respectively, Q_{Dis} is the baseline energy input by the solvent and sample cell without nanoparticles, I is the laser power, and A_λ is the absorbance of the $CuMo_2S_3$ NCs at 808 nm. Based on the obtained data (Figure S4 a and b), the η value of $CuMo_2S_3$ NCs was calculated to be ~45.8%.

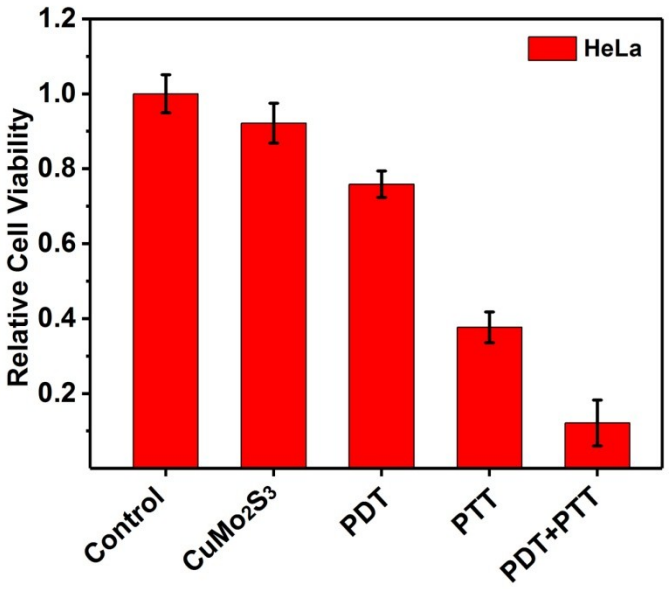

Fig. S5 Relative viabilities of HeLa cell after different treatments, including the untreated group, only $CuMo_2S_3$ group, only PDT group, only PTT group and PDT/PTT combined group.

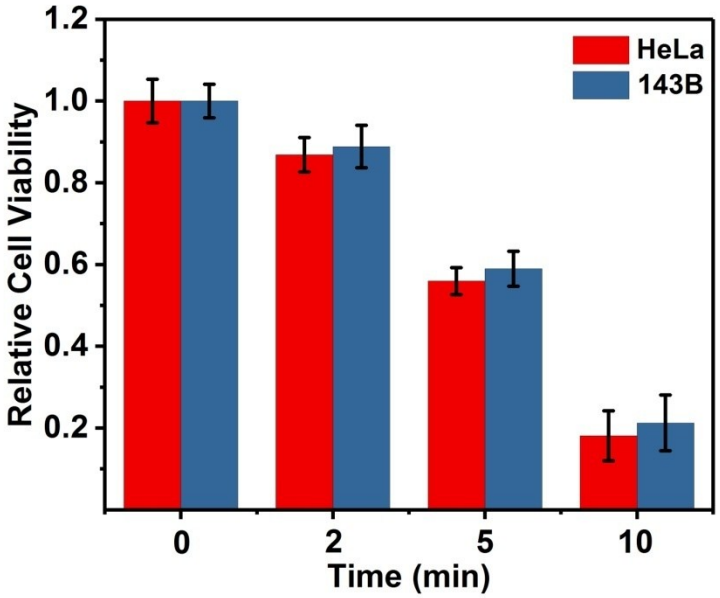

Fig. S6 Relative viabilities of HeLa and 143B cells incubated with $CuMo_2S_3$ NCs under different irradiation duration of 808 nm laser.

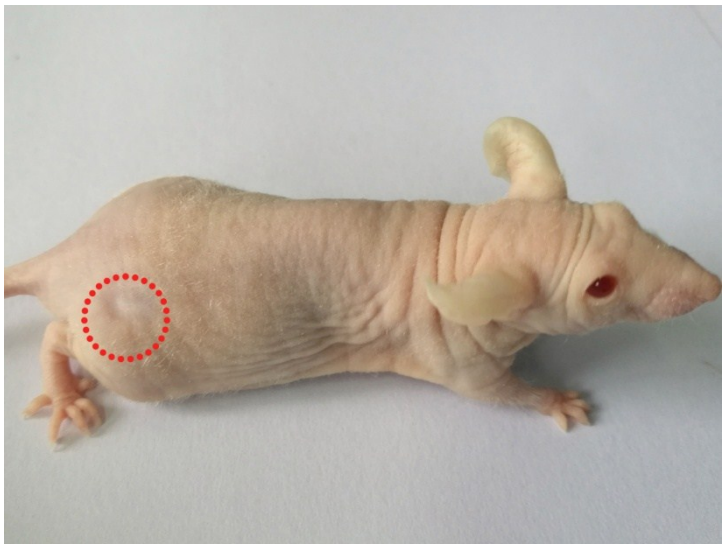

Fig. S7 Photo of $CuMo_2S_3$ + NIR group mouse at 40th day after treatments, the tumor location was marked with red dotted line circle.

1 B. Li, Y. Zhang, R. Zou, Q. Wang, B. Zhang, L. An, F. Yin, Y. Hua and J. Hu, *Dalton Trans.*, 2014, **43**, 6244-6250.