

Supporting Information

Near infrared dye-coated silver nanoparticle/carbon dot nanocomposite for targeted tumor imaging and enhanced photodynamic therapy

Rongjun Liu,^{a,b} Zhengmin Yang,^a Liangliang Zhang,^{*,a} Jingjin Zhao,^a Cheng Hou^a and Shulin

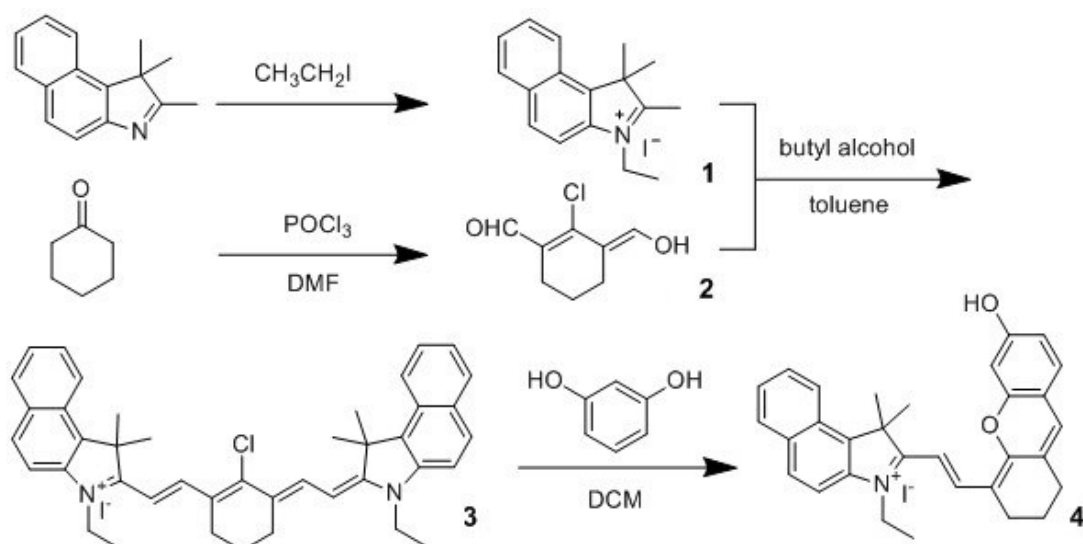
Zhao^{*,a}

^a State Key Laboratory for the Chemistry and Molecular Engineering of Medicinal Resources,

Guangxi Normal University, Guilin, 541004, China

^b Guangxi Key Laboratory of Agricultural Resources Chemistry and Biotechnology, College of

Chemistry and Food Science, Yulin Normal University, Yulin, 537000, China



Scheme S1. Synthetic routine of CyOH.

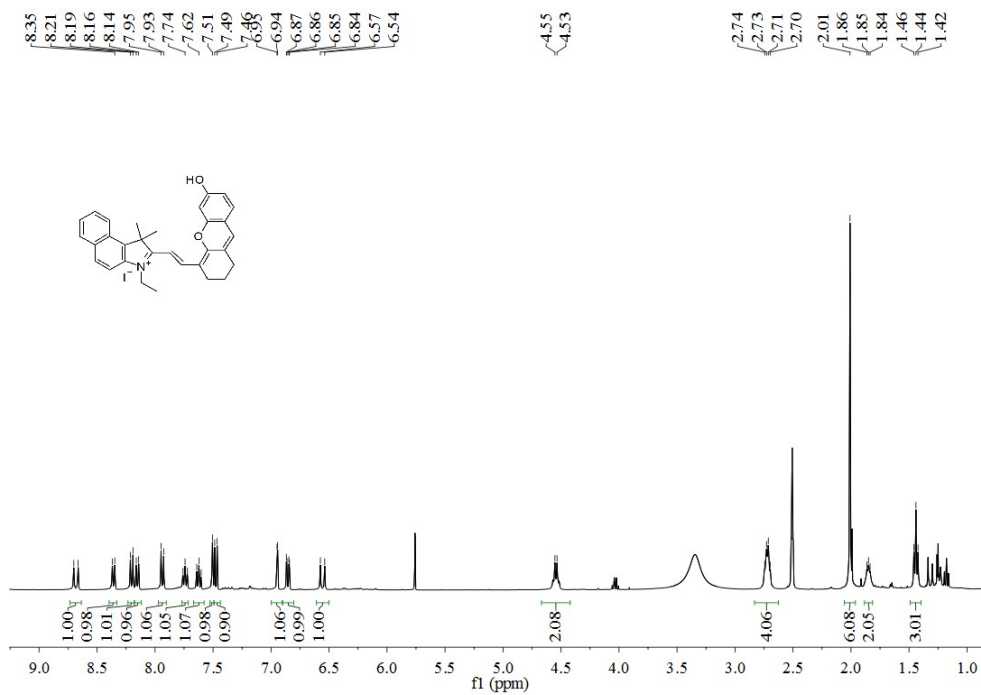


Figure S1. ¹H NMR spectrum of CyOH in DMSO.

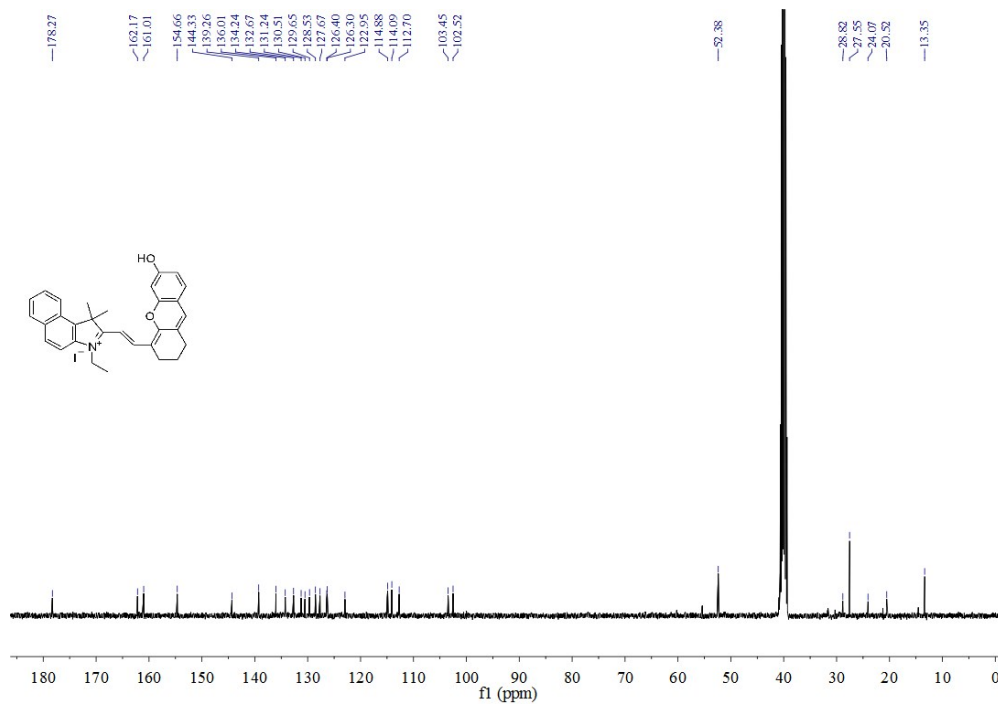


Figure S2. ¹³C NMR spectrum of CyOH in DMSO.

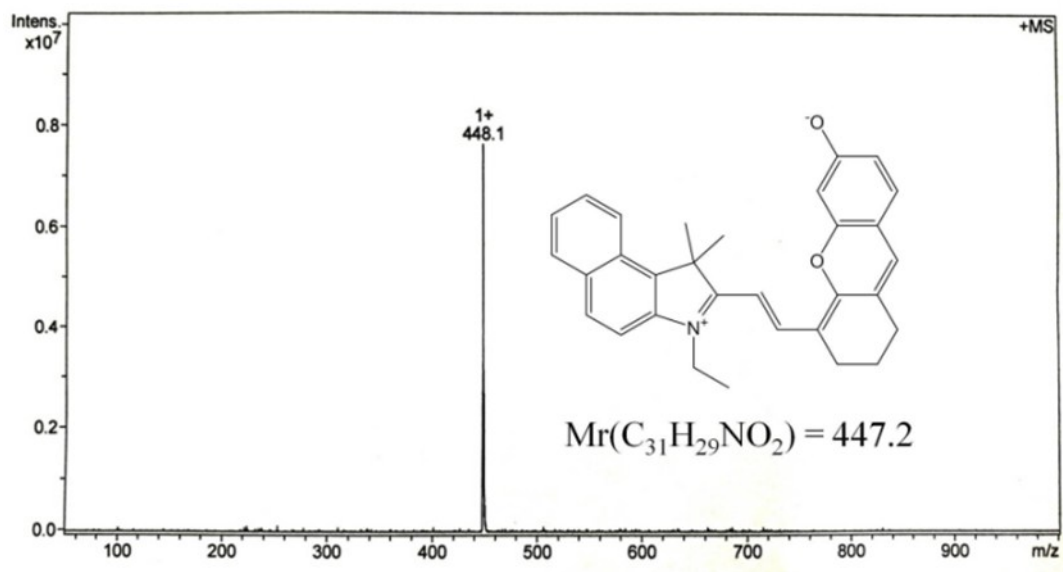


Figure S3. MS spectrum of CyOH.

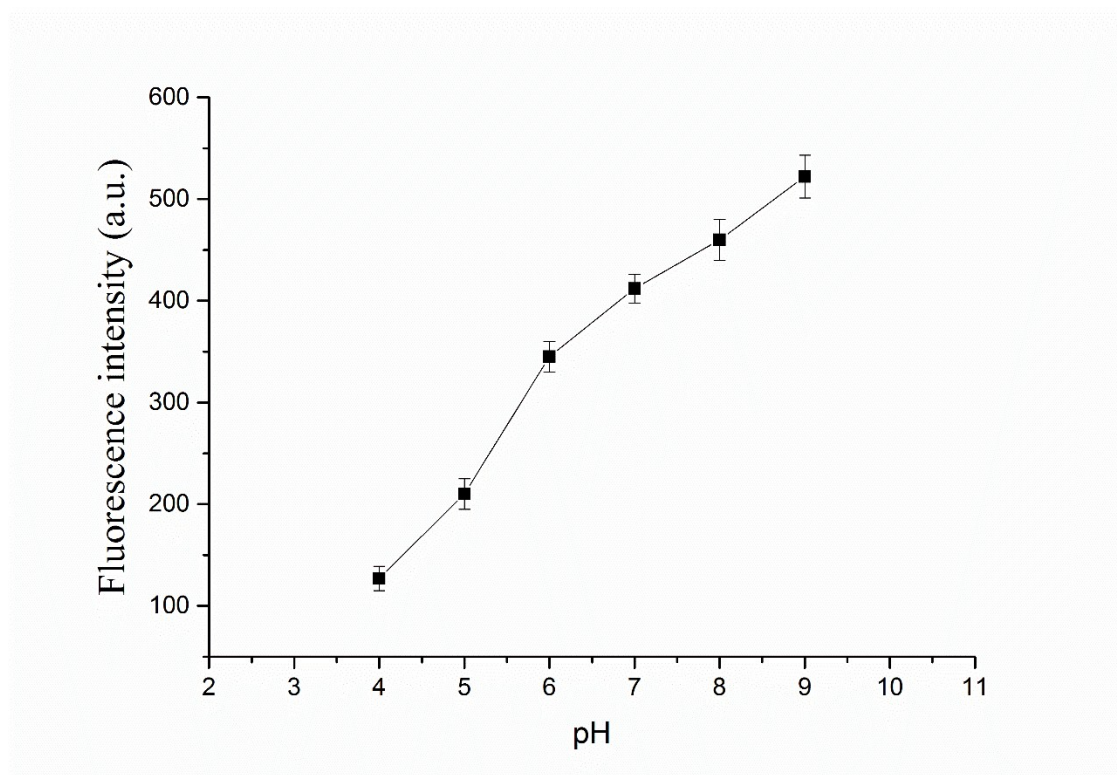


Figure S4. The fluorescence intensity of CyOH–AgNP/CD ($\lambda_{ex} = 633$ nm) in ethanol/Tris-HCl buffer solution (1:1 v/v) in the range of pH values from 3 to 9.

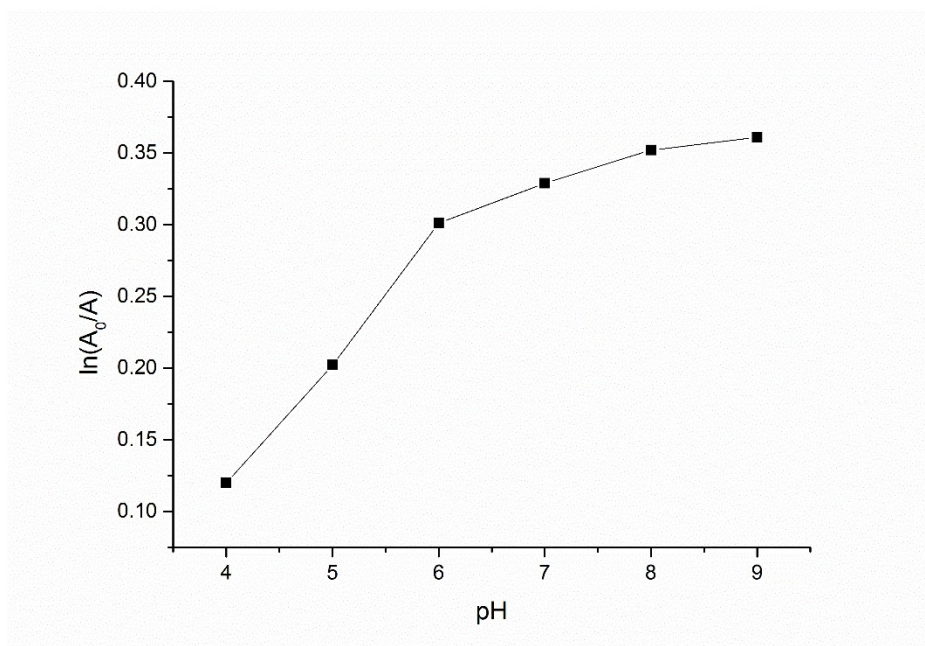


Figure S5. The decomposition rate of DPBF by CyOH–AgNP/CD in the range of pH values from 3 to 10 (660 nm laser for 2 min).

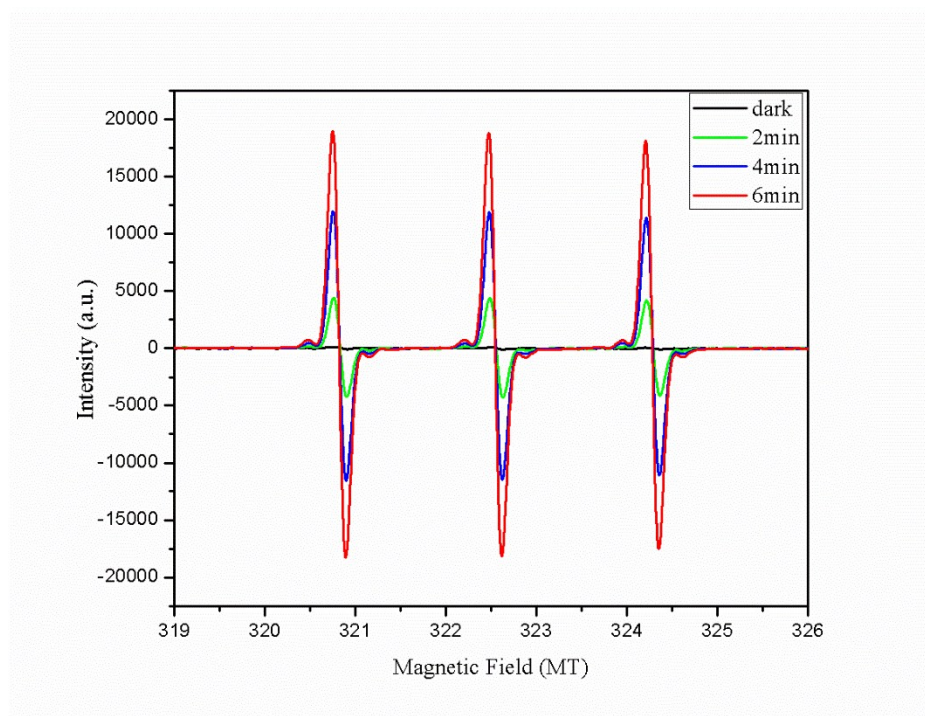


Figure S6. The EPR spectra of $^1\text{O}_2$ produced in the presence of CyOH–AgNP/CD by after irradiation with a 660 nm laser.

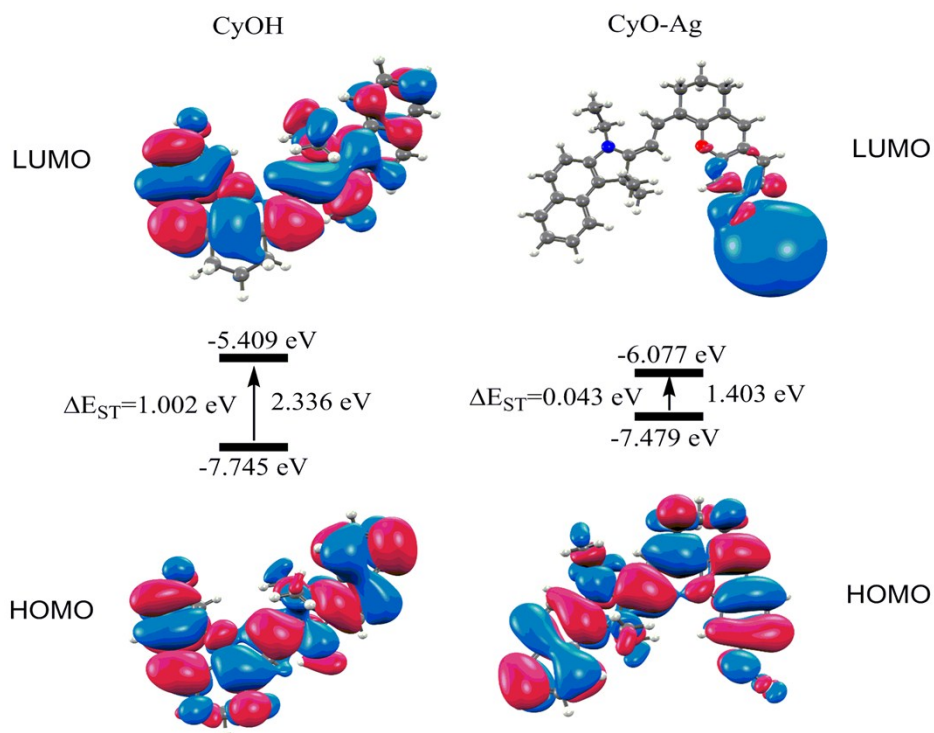


Figure S7. Frontier molecular orbital distribution, energy gaps (ΔE_{ST}) between S1 and T1 for ligand (left) and Ag^+ -ligand (right) calculated by TD-DFT.

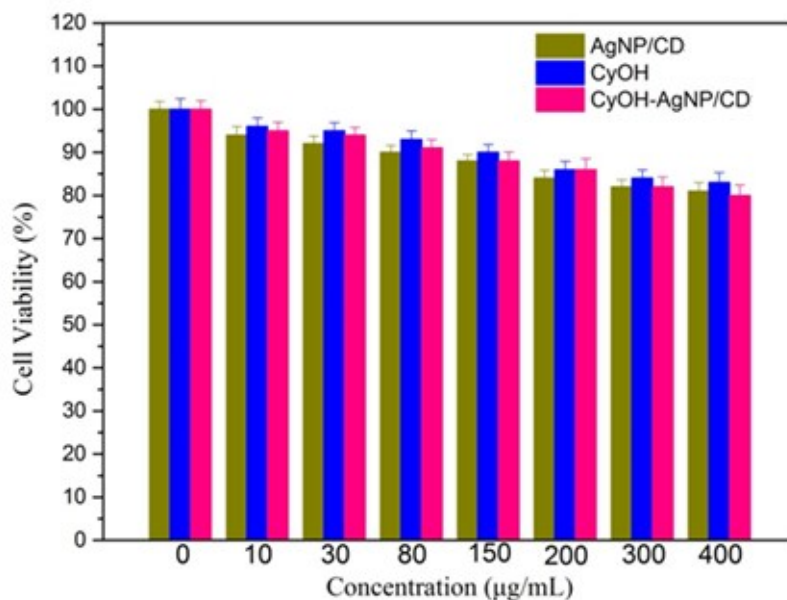


Figure S8. Relative viability of 4T1 cell incubated with various concentrations of AgNP/CD, CyOH and CyOH-AgNP/CD.

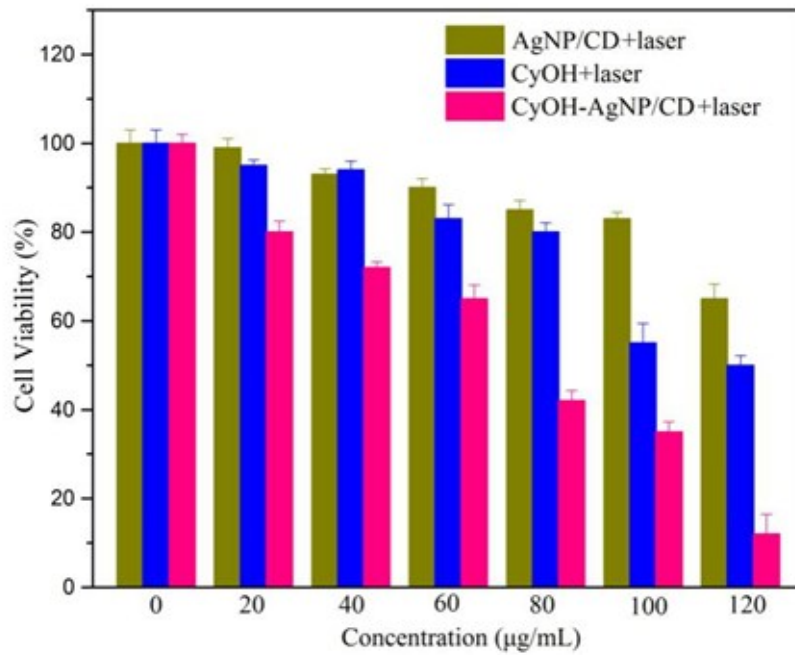


Figure S9. Relative viability of 4T1 cell incubated with various concentrations of AgNP/CD, CyOH and CyOH-AgNP/CD with irradiation using a 660 nm laser (50 mW/cm², 5 min).

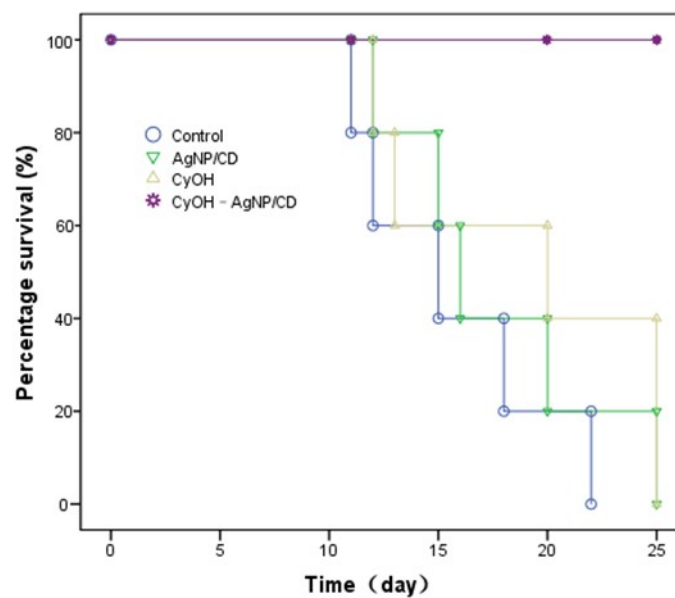


Figure S10. Mice survival curves during the treatment of Control, AgNP/CD, CyOH and CyOH-AgNP/CD groups.

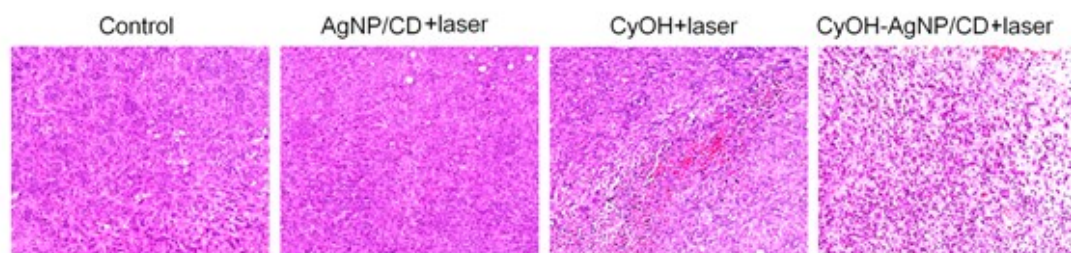


Figure S11. H&E-stained images of tumor tissues from sacrificed mice in the four groups after treatment for 20 days.

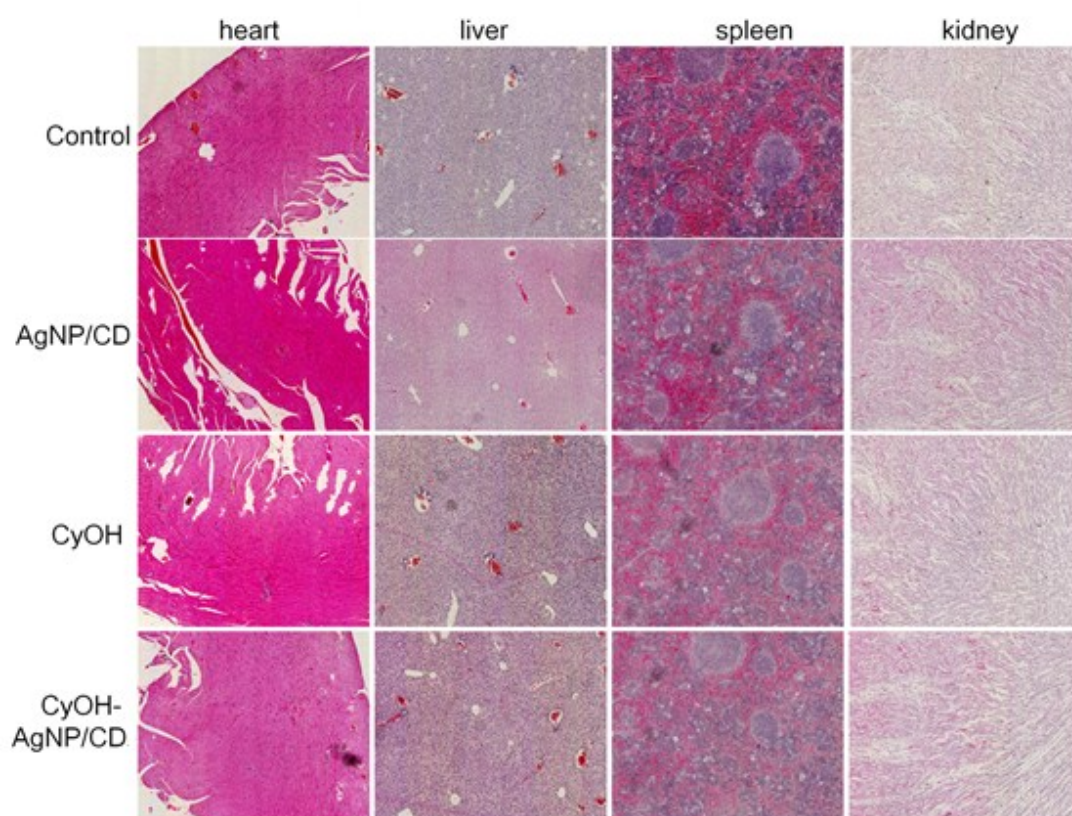


Figure S12. H&E-stained images of tissue slides for main organs (heart, liver, spleen and kidney) from sacrificed mice in the four groups after treatment for 20 days.

Table S1. Triplet and singlet excitation energy of ligand and Ag-ligand calculated by TD-DFT at the B3LYP/6-31G level.

	State	E(eV)	ΔE_{ST} (eV)
Ligand	S1	2.1883	1.0022
	S2	2.6441	
	T1	1.1861	
	T2	2.1529	
Ag-Ligand	S1	0.9724	0.0429
	S2	1.7087	
	T1	0.9295	
	T2	1.1960	