

Electronic Supplementary Information (ESI)
for
**Surface Ligand Coordination Induced Self-assembly of
Nanohybrid for Efficient Photodynamic Therapy and
Imaging**

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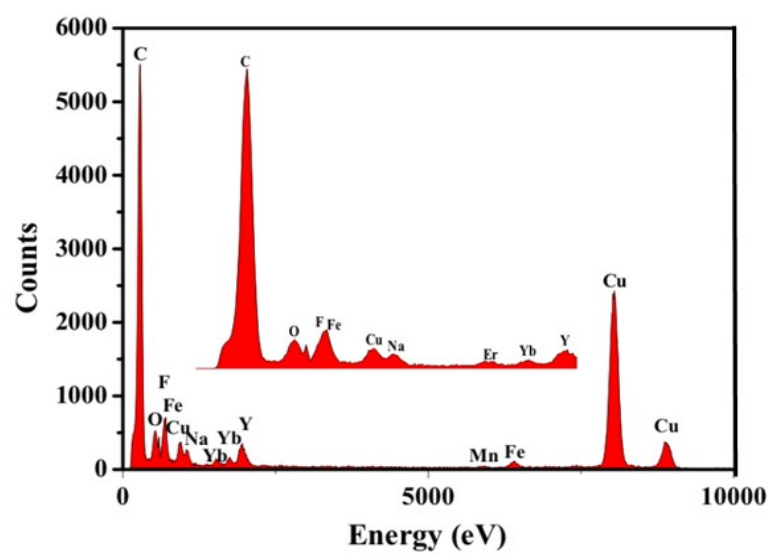


Fig. S1 The EDS of UCNPs@MF (inset: the enlarged area of EDS from 0 keV to 2 keV)

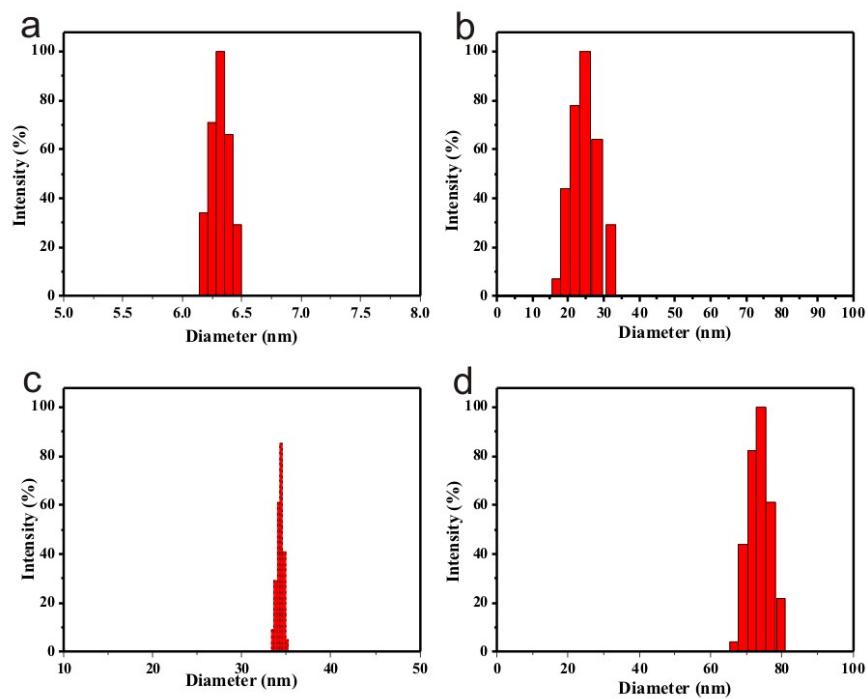


Fig. S2 Size distribution of (a) MnFe_2O_4 NPs, (b) $\text{NaYF}_4\text{:Yb/Er}$ NPs, (c) $\text{NaYF}_4\text{:Yb/Er@NaYF}_4$ NPs and (d) UCNPs@MF HNPs measured by dynamic light scattering.

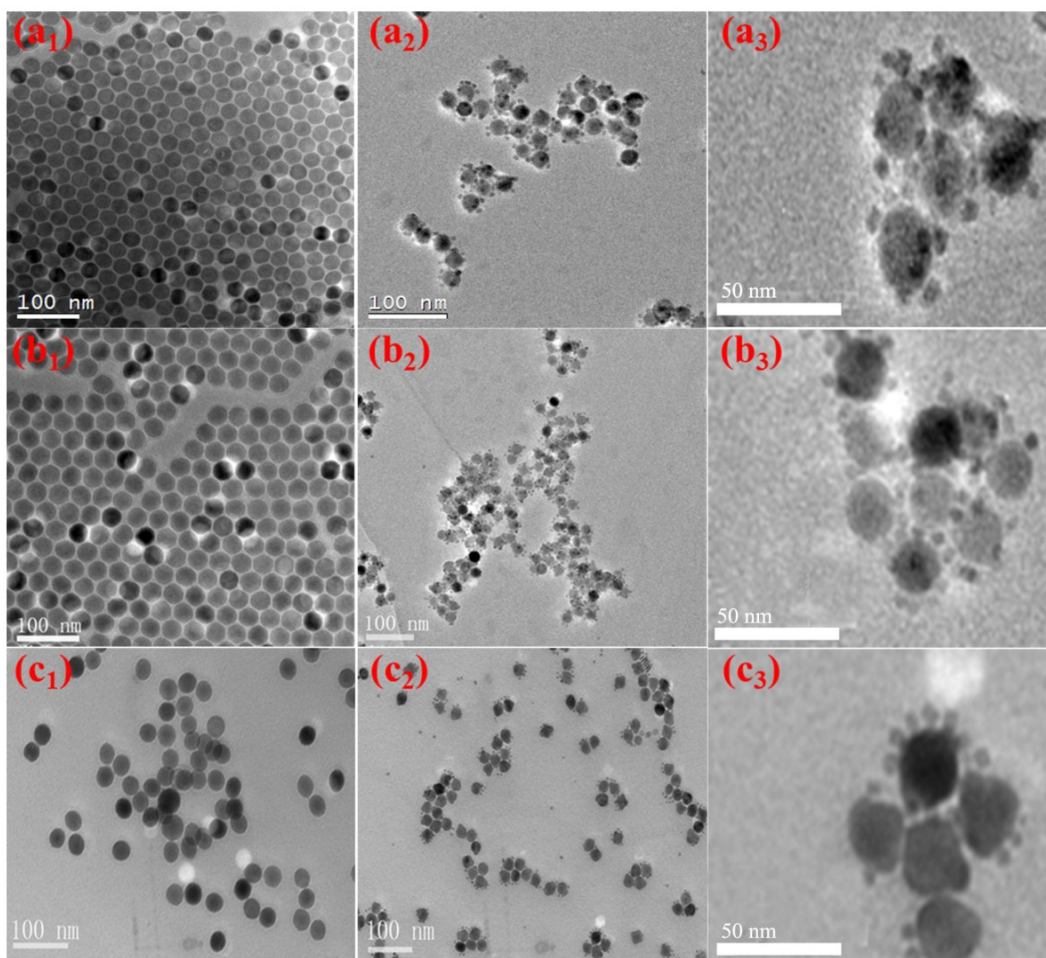


Fig. S3 TEM images of a₁) NaYF₄:Yb/Er@NaYF₄ NPs, b₁) NaYF₄:Yb/Er@NaGdF₄ NPs, c₁) NaYF₄:Yb/Er@NaNdF₄ NPs and a₂-a₃) UCNPs@MF HNPs, b₂-b₃) NaYF₄:Yb/Er@NaGdF₄@MnFe₂O₄ NPs and c₂-c₃) NaYF₄:Yb/Er@NaNdF₄@MnFe₂O₄ NPs at different magnifications.

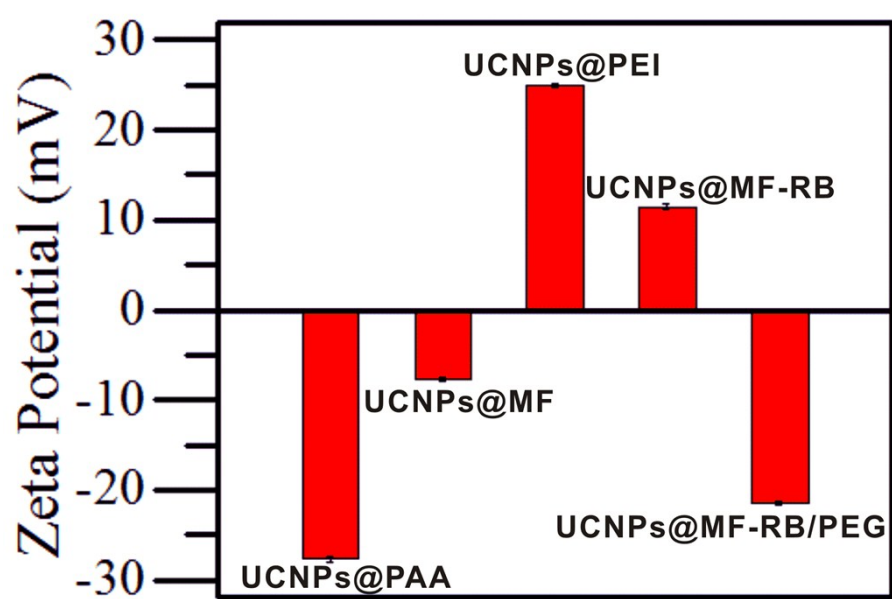


Fig. S4 Zeta potentials of the intermediate and final products.

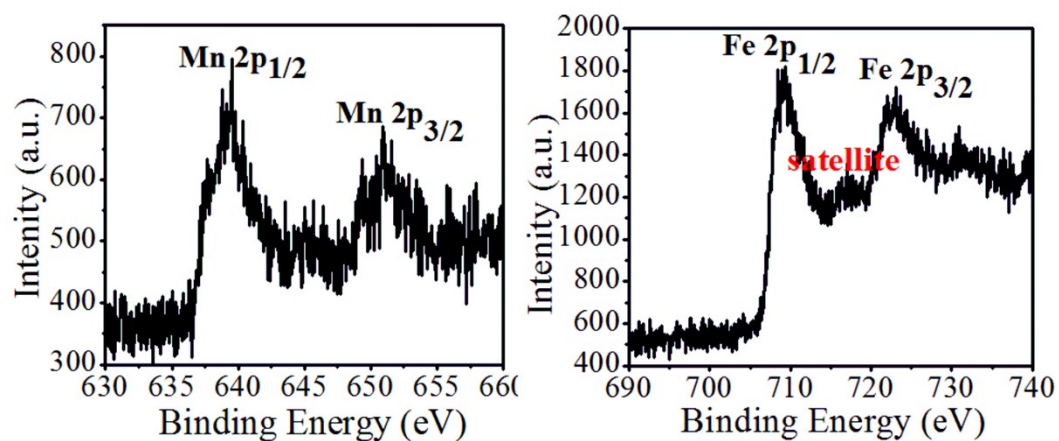


Fig. S5 The high resolution XPS data for the MnFe_2O_4 in the (a) Mn and (c) Fe regions.

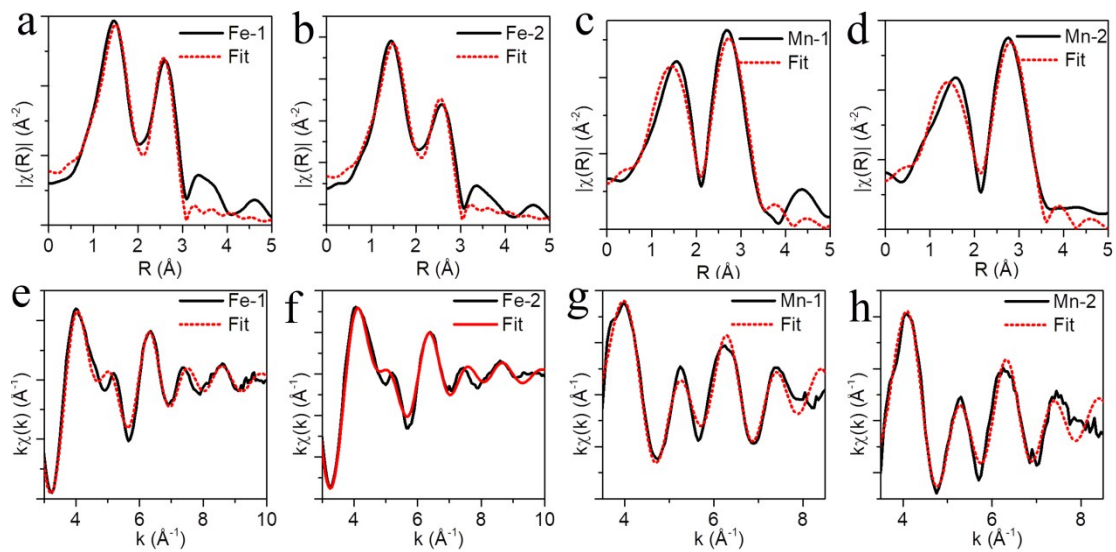


Fig. S6 EXAFS R-space and k-space fitting results of Fe (a, e) in MF NPs, (b, f) in UCNPs@MF HNPs; Mn (c, g) in MF, (d, h) in UCNPs@MF HNPs.

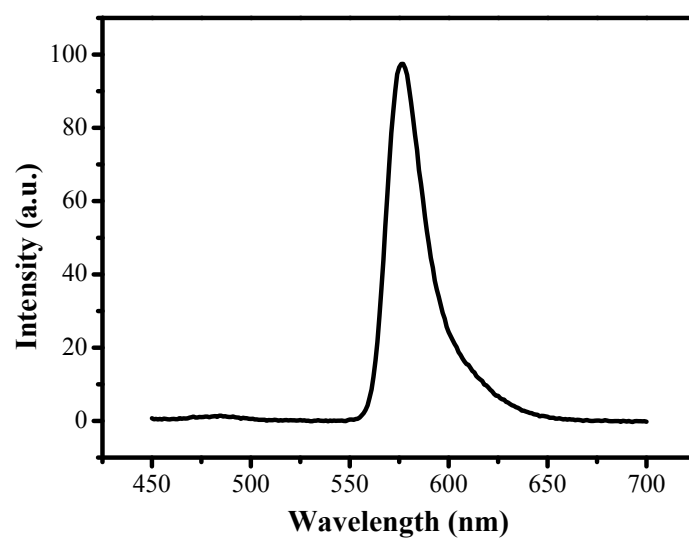


Fig. S7 The emission spectrum of RB.

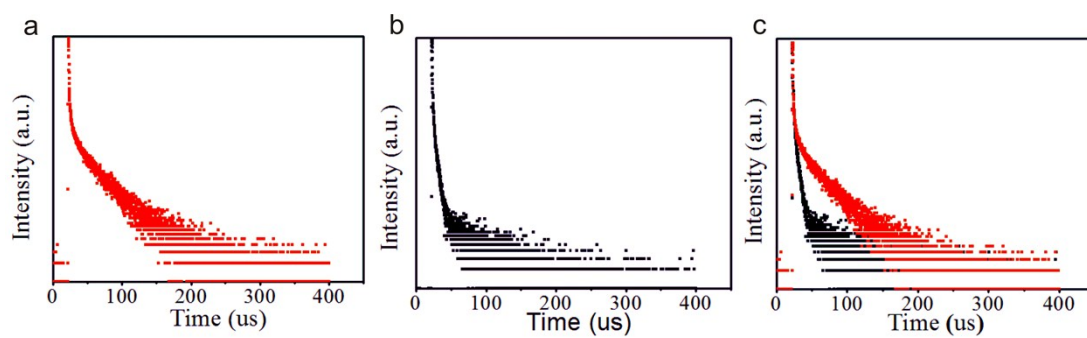


Fig. S8 The decay curves at the wavelength of 540 nm for (a) UCNPs@MF, (b) UCNPs@MF-RB/PEG and (c) combined decay curves. Excitation by 980 nm laser.

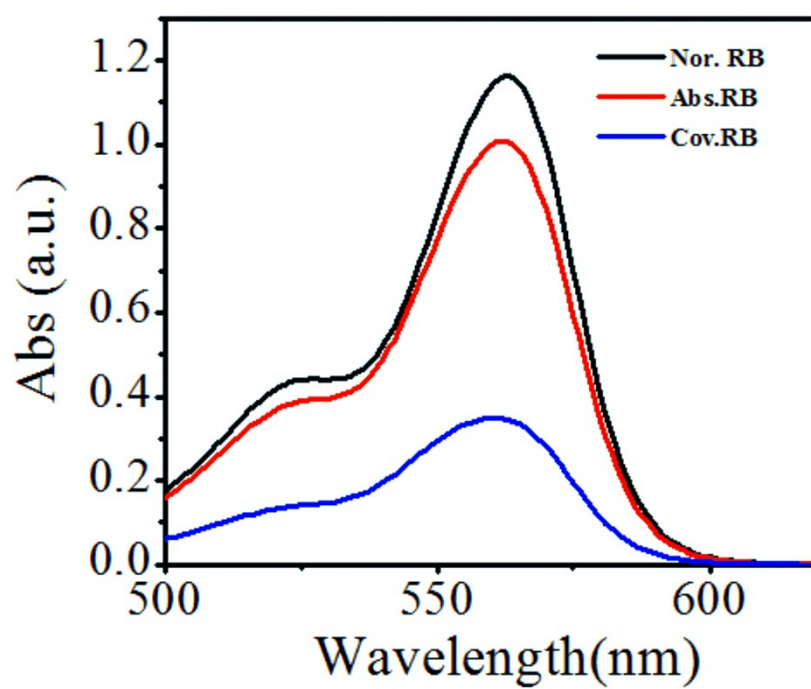


Fig. S9 UV-vis spectra of RB (black). RB eluate after washing with DMSO three times from the physically adsorbed UCNPs@MF (red) and covalently bonded from UCNPs@MF-RB/PEG.

Table S1. Comparison of EXAFS curve fit parameters of coordination number (CN), bonding distance (R), Debye-Waller factor (σ^2), and shift in adsorption edge energy (ΔE_0) for each shell of MF (Fe-1 and Mn-1) and UCNPs@MF (Fe-2 and Mn-2).

Sample	shell	C.N.	R (Å)	ΔE (eV)	σ^2 (Å ⁻²)	R factor
Mn-1	Mn-O	3.7±0.9	2.0±0.02	-11.0±2.5	0.007±0.003	0.015
	Mn-Fe(Mn)	7.7±2.5	3.4±0.03			
Mn-2	Mn-O	4.5±0.8	2.0±0.04	-7.4±3.7	0.011±0.002	0.016
	Mn-Fe(Mn)	11.0±2.5	3.4±0.04			
Fe-1	Fe-O	3.6±0.4	3.0±0.01	3.7±1.0	0.011±0.002	0.009
	Fe-Fe(Mn)	5.2±1.0	3.0±0.01			
Fe-2	Fe-O	5.3±0.7	1.9±0.02	3.9±1.2	0.011±0.003	0.011
	Fe-Fe(Mn)	5.9±1.5	3.0±0.02			

Table S2. The lifetimes at the wavelength of 545 nm for UCNPs@MF and UCNPs@MF-RB/PEG.

	τ_1 (μs)	τ_2 (μs)	τ (μs)
UCNPs@MF	19.31 (11.55%)	91.92 (88.45%)	83.53
UCNPs@MF-RB/PEG	10.12(66.81%)	106.18 (33.19%)	42.00

The average lifetime was calculated according to the equation $\langle\tau\rangle = \frac{\sum A_i \tau_i^2}{\sum A_i \tau_i}$, where τ

is the component decay times and A_i is weighed amplitudes.