Electronic Supplementary Information

Core-shell materials bearing iron (II) carbonyl units and their CO-release via

upconversion process

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Fig. S1 Characterizations of β-NaYF₄:Yb³⁺/Er³⁺ UCNPs: (a) and (b) TEM images, (c) hydrodynamic diameter distribution in cyclohexane, (d) X-ray diffraction pattern (A JCPDS file of standard β-NaYF₄:Yb³⁺/Er³⁺ powder is given as a reference).



Fig. S2 Photograph of UCNPs which was dispersed in cyclohexane.



Fig. S3 Magnification TEM images of the nanoparticles at different stages of the onepot formation reaction: (a) UCNPs, (b) UCNPs@SiO₂, (c) UCNPs@SiO₂-SH, (d) UCNPs@SiO₂-CORMs.



Fig. S4 SEM images of UCNPs (a), UCNPs@SiO₂ (b), UCNPs@SiO₂-SH (c), UCNPs@SiO₂-CORMs (d).



Fig. S5 Infrared spectral variation in DMSO / D2O (1:1) in dark.



Fig. S6 Diameter sizes of the UCNPs@SiO₂-CORMs nanomaterials determined by dynamic light scattering test in different media within 24 h. For the water medium and DMEM, 10% of DMSO was added to disperse the materials.



Fig. S7 FTIR spectra of $[(\eta^5-Cp)Fe(\mu-CO)(CO)]_2$ (blue) and complex 1 (red) in CH_2Cl_2



Fig. S8 ¹H NMR spectrum of $[(\eta^5-Cp)Fe(\mu-CO)(CO)]_2$ in CDCl₃



Fig. S9 ¹H NMR spectrum of complex 1 in $CDCl_3$

Table S1. Particle size distribution of UCNPs (1), UCNPs@SiO₂ (2), UCNPs@SiO₂-

	1	2	3	4
Diameter / nm	66 nm	89 nm	104 nm	119 nm

SH (3), UCNPs@SiO₂-CORMs (4) in ethanol solvent.