Electronic Supplementary Information

Oxygen and pH responsive theragnostic liposome for early-stage diagnosis and photothermal therapy of solid tumour

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Supplementary Figures

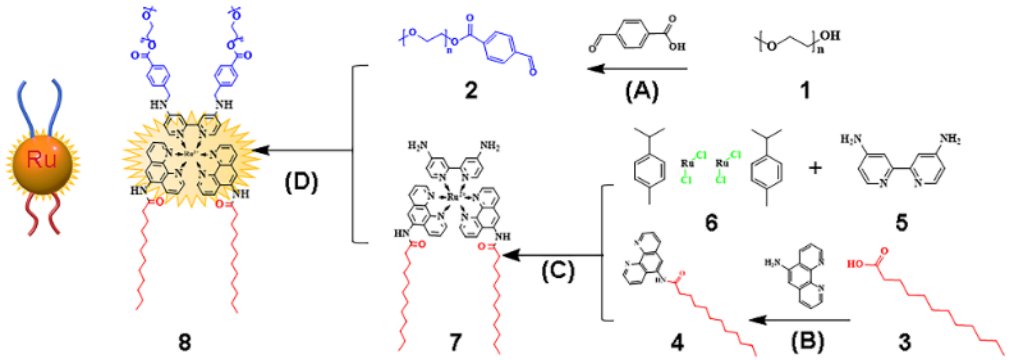

Figure S1. The synthetic route of amphiphilic ruthenium complex, i.e. C_{12}-RuA_2D-PEG_{2K}. (A) DCC, DMAP, DCM, IPA. (B) EDC, DMAP, DCM. (C) Ethanol, acetone. (D) Methyl alcohol. 1. $mPEG_{2K}$, 2. $mPEG_{2K}$-CHO, 3. Lauric acid, 4. C_{12}-grafted phenanthroline, 5. 4,4'-Diamino-2,2'-bipyridine, 6. Dichloro(p-cymene)ruthenium(II) dimer, 7. C_{12}-RuA_2D, 8. C_{12}-RuA_2D-PEG_{2K}.

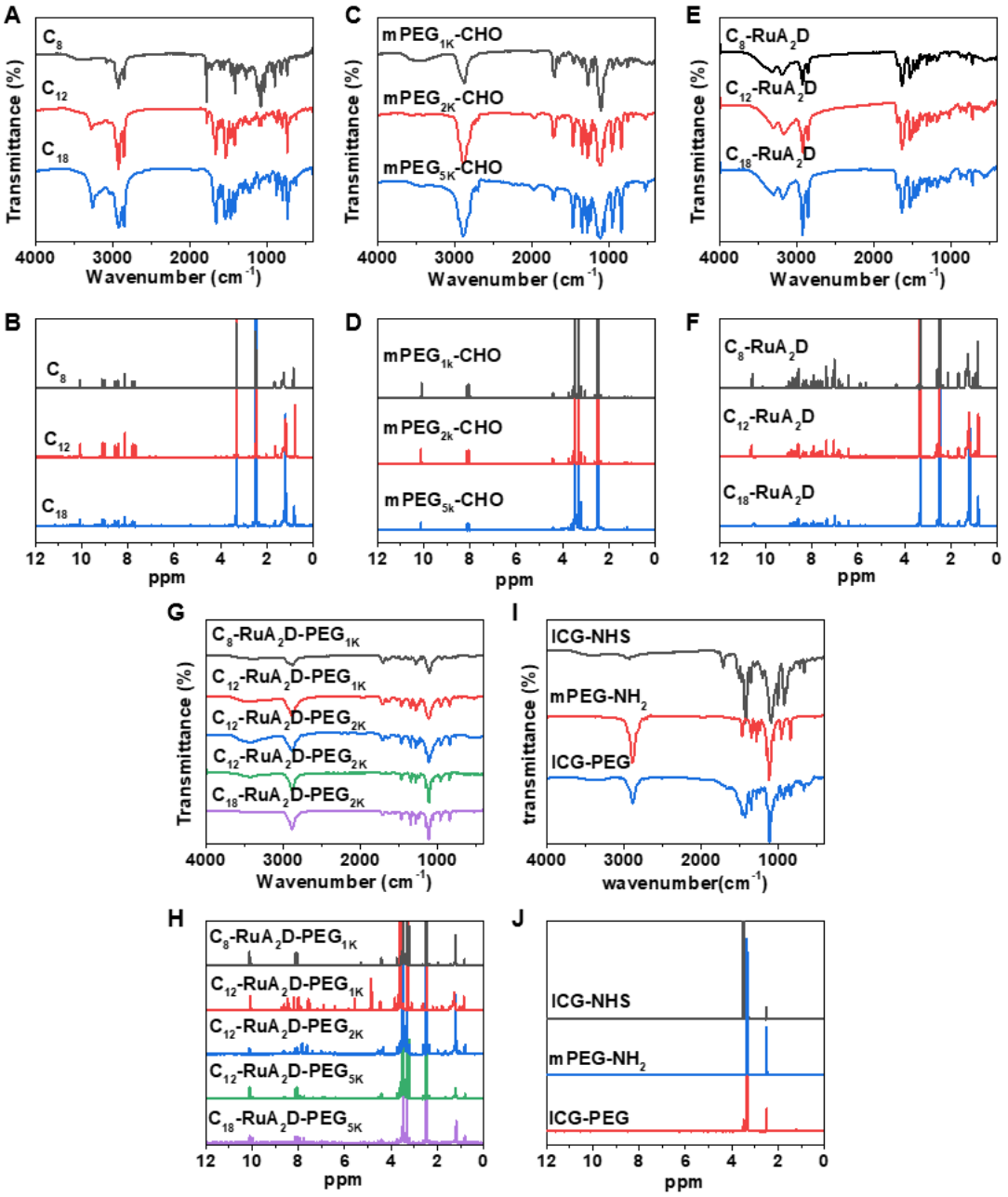

Figure S2. FTIR spectra (A, C, E, G) and ^{1}H NMR spectra (B, D, F, H) of alkyl chain (C_8, C_{12}, C_{18}) modified phenanthroline, i.e. C_n-grafted phenanthroline (A, B), benzaldehyde caped mPEG (mPEG-CHO) with different molecular weight (C, D), alkyl chain (C_8, C_{12}, C_{18}) modified ruthenium complex, i.e. C_n-RuA_2D (E, F), amphiphilic ruthenium complex, i.e. C_n-RuA_2D-PEG (G, H) and the reagent as well as the product of PEGylated ICG, i.e. ICG-PEG (I, J).

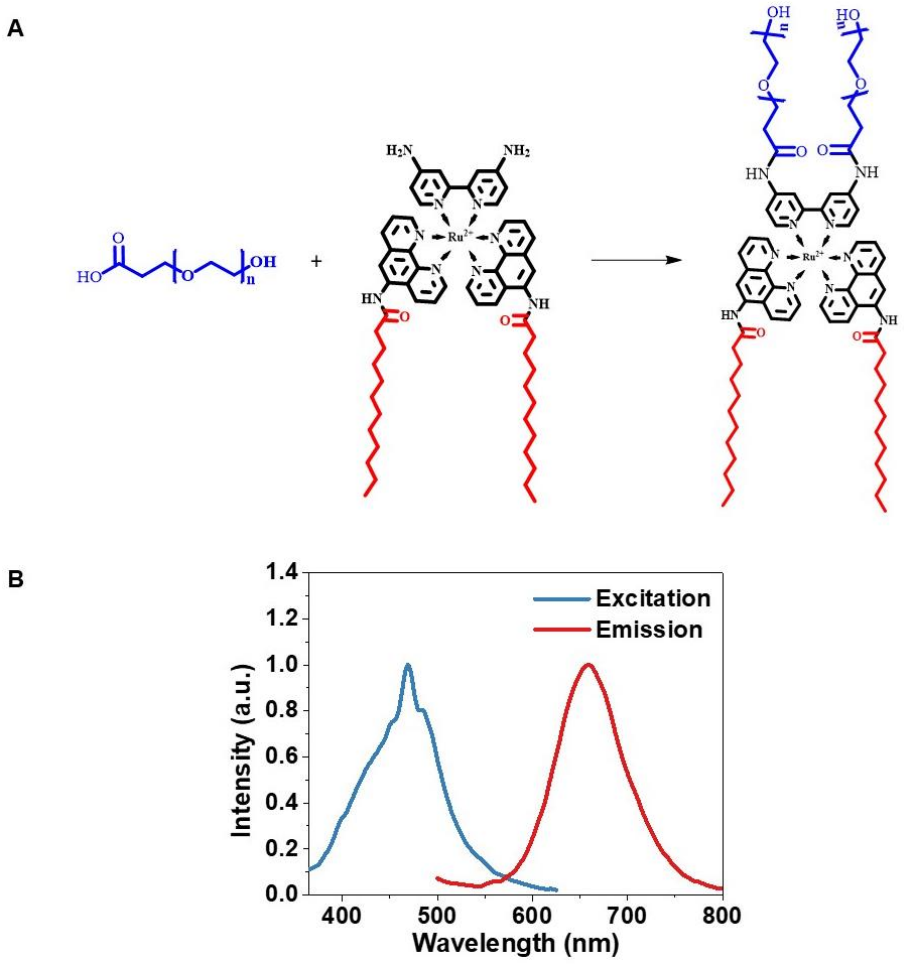

Figure S3. (A) The synthetic route of pH insensitive PEGylated C_{12}-RuA_2D. (B) Excitation and emission spectra of the pH insensitive PEGylated C_{12}-RuA_2D.

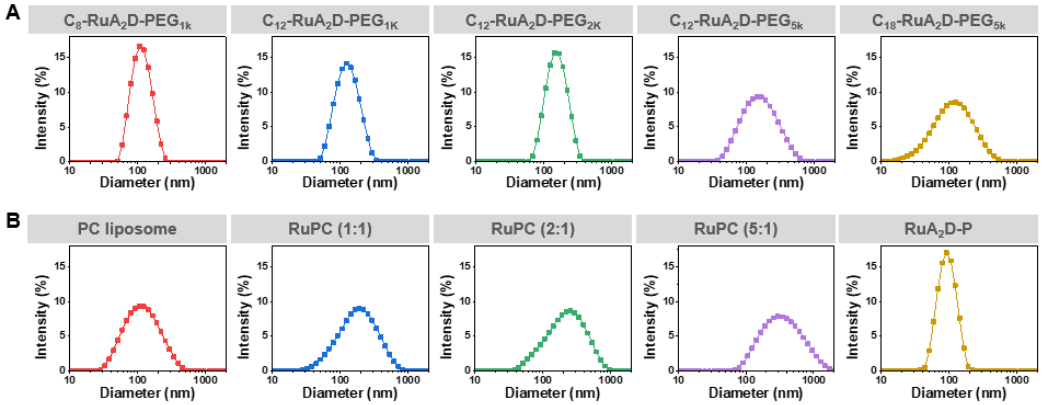

Figure S4. (A) DLS of C_n-RuA_2D-PEG self-assemblies with different alkyl and PEG chain lengths. (B) DLS of phosphatidylcholine (PC) liposome, C_{12}-RuA_2D-PEG_{2K} co-assemblies (RuPC) with different ruthenium complex-to-PC weight ratio, and the sonicated dispersion of C_{12}-RuA_2D-PEG_{2K} (RuA_2D-P). In the co-assemblies, cholesterol was added at a weight ratio of 0.1 to the mass of PC.

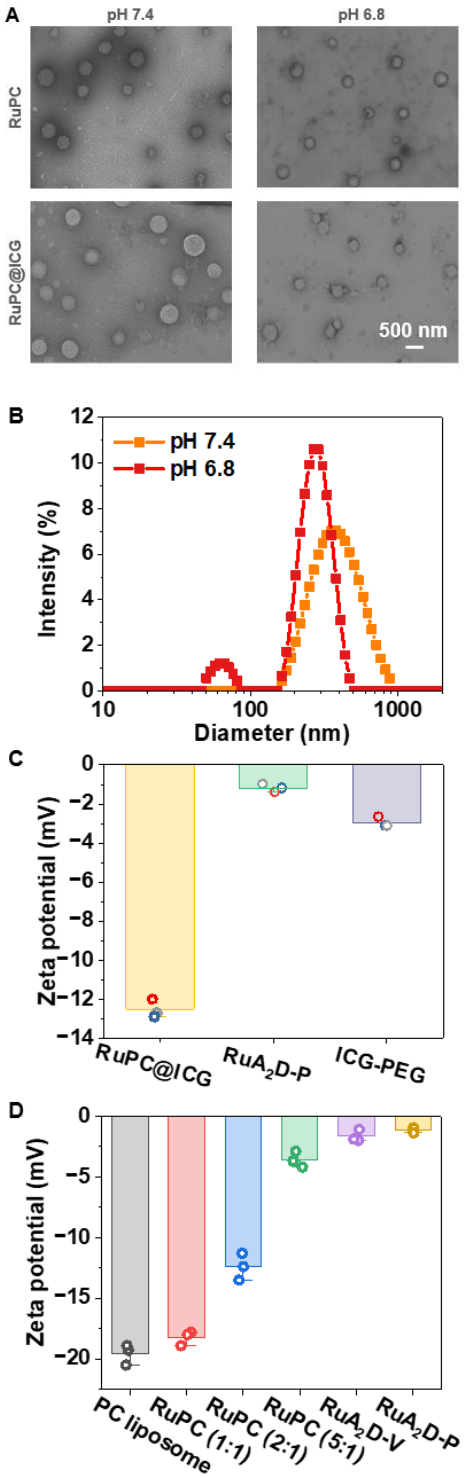

Figure S5. (A) TEM of RuPC and ICG-PEG loaded RuPC (RuPC@ICG) prepared from PBS dispersion at pH 7.4 or pH 6.8. (B) DLS of RuPC@ICG in PBS at pH 7.4 or pH 6.8. (C) Zeta potentials of RuPC@ICG, ICG-PEG and RuA_2D-P in PBS (pH 7.4). (D) Zeta potentials of self-assembled, co-assembled C_{12}-RuA_2D-PEG_{2K} and RuA_2D-P.

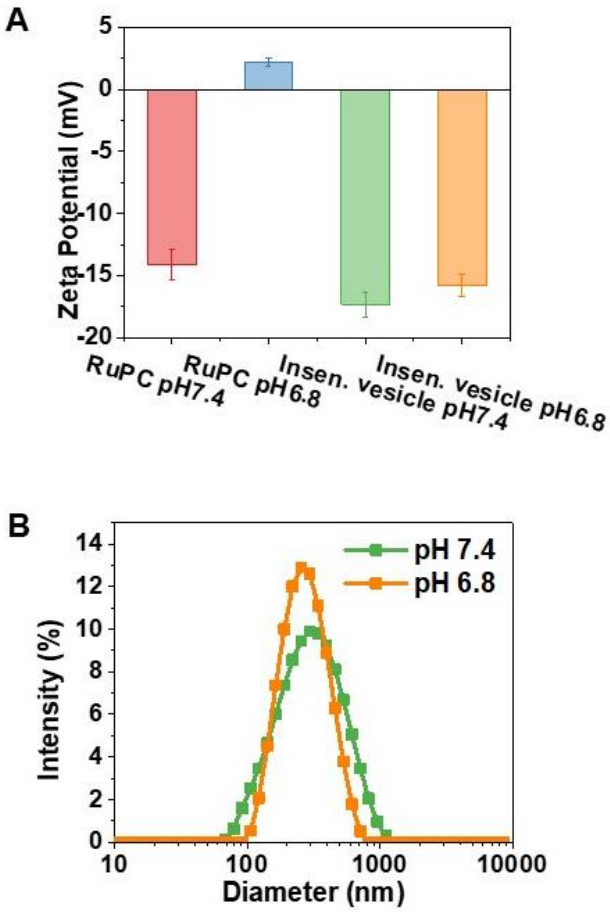

Figure S6. (A) Zeta potentials of RuPC and pH insensitive vesicle formed by pH insensitive PEGylated C_{12}-RuA_2D and PC in PBS at pH 7.4 or pH 6.8. (B) DLS of pH insensitive RuPC vesicle in PBS at pH 7.4 or pH 6.8.

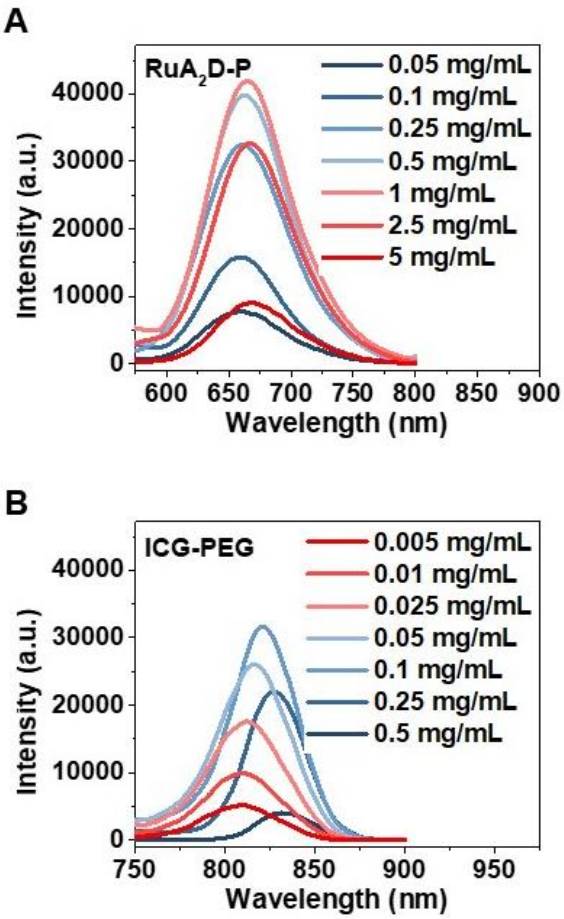

Figure S7. Fluorescence spectra of RuA_2D-P (A) and ICG-PEG (B) in PBS (pH 7.4) at different concentrations.

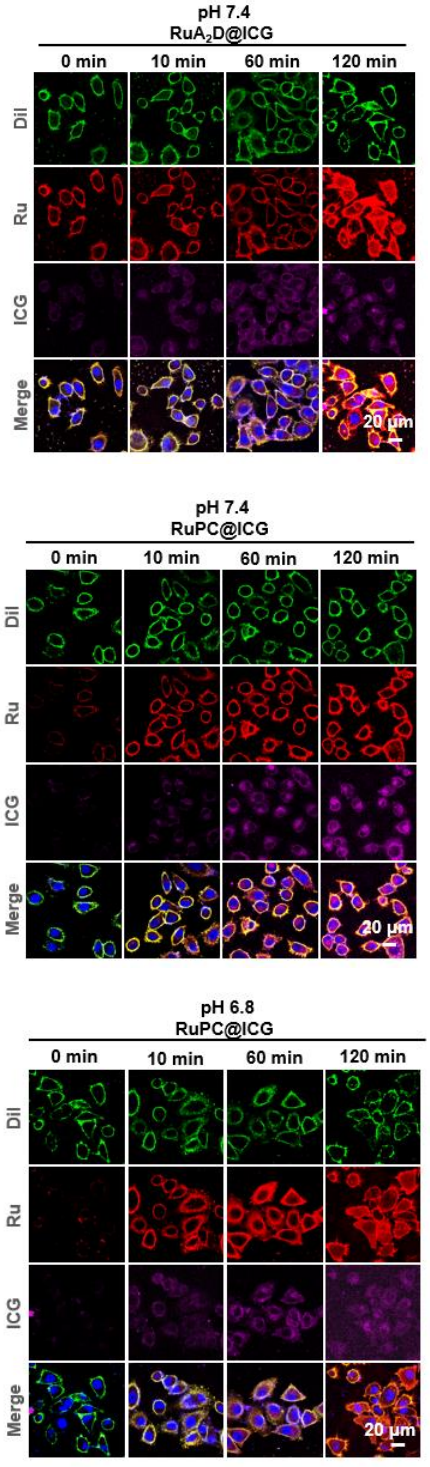

Figure S8. LCSM images of HeLa cells incubated with ICG-PEG encapsulated self-assembled C_{12}-RuA_2D-PEG_{2K} vesicles (RuA_2D@ICG) and RuPC@ICG for different times at pH 7.4 or 6.8. The concentration of RuA_2D@ICG and RuPC@ICG was 200 μg mL^{-1}.

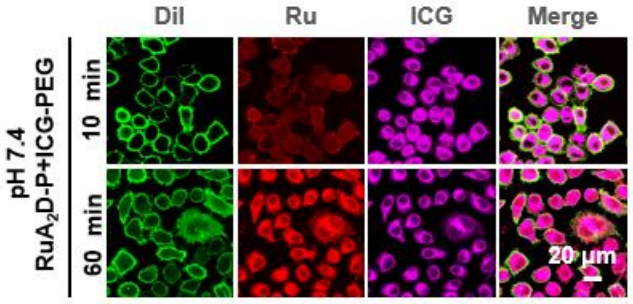

Figure S9. LCSM of HeLa cells incubated with the mixture of RuA_2D-P (200 μg mL^{-1}) and ICG-PEG (50 μg mL^{-1}) for different time at pH 7.4.

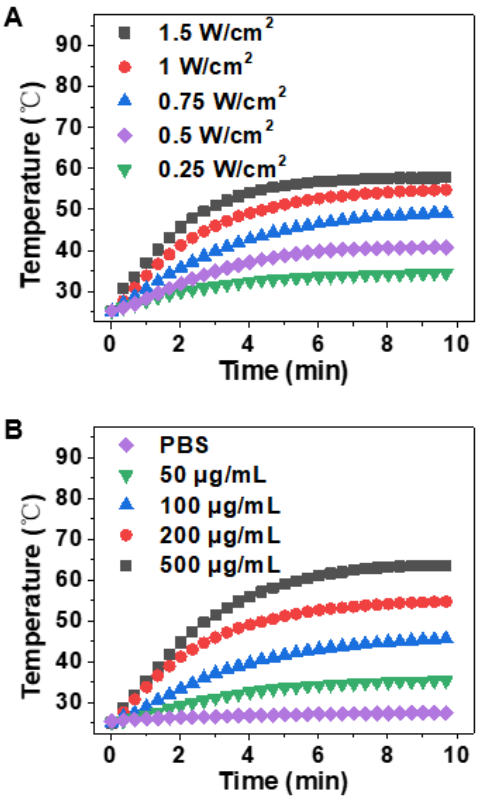

Figure S10. Influence of irradiation power (A) and sample concentration (B) on the photothermal effect of RuPC@ICG liposome in PBS under 808 nm excitation. (A) The concentration of ICG-PEG in RuPC@ICG dispersion was kept at 200 μg mL^{-1}. (B) The irradiation powder was 1 W cm^{-2}.

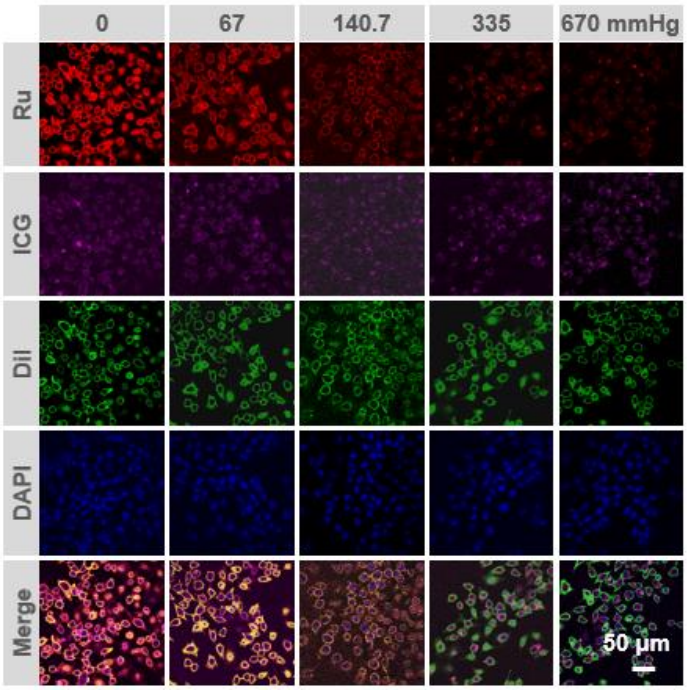

Figure S11. LCSM images HeLa cells incubated with RuPC@ICG liposome (200 μg mL^{-1}) in culture medium (pH 7.4) with different oxygen partial pressure.

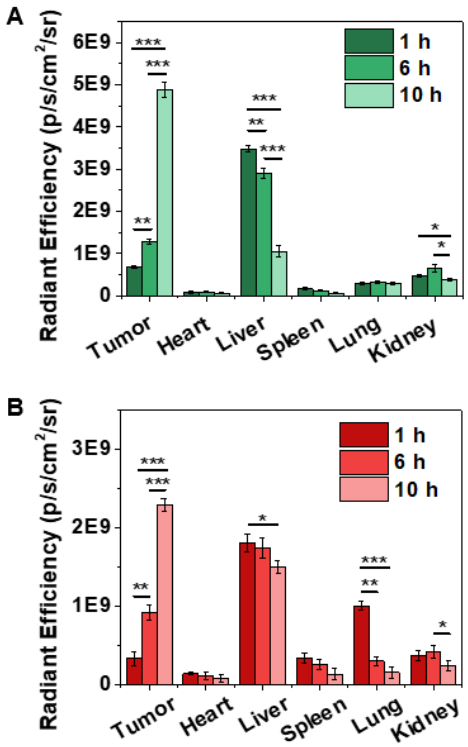

Figure S12. Quantitative analysis of *ex vivo* emission intensity of ICG (A) and ruthenium (B) in major organs and tumour tissue of tumour bearing mice (n = 3) after being dosed by RuPC@ICG *via* intravenous injection for 1 h, 6 h and 10 h.