Supporting Information

Phosphonated mesoporous silica nanoparticles bearing ruthenium complexes used as molecular probe for tracking oxygen levels in cells and tissues

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Table S1. Weight Loss of Particles in Each Step in Scheme 1.[a]

	pM-Ru-48-100	pM-Ru-41-100	pM-Ru-48-50
Particle I	45%	43%	29%
Particle II	40%	35%	28%
Particle III	11%	5.2%	8.8%
Particle IV	16%	15%	18%

[a]Weight loss was estimated by using thermogravimetric analysis.

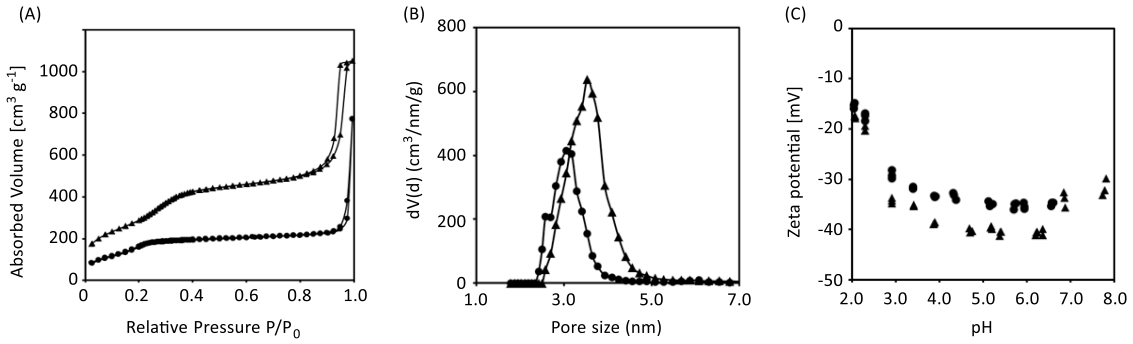

Figure S1. (A) N_2 physisorption isotherms of pM-Ru-41-100 (triangle) and pM-Ru-48-50 (circle). The analysis was conducted at –196 ˚C. (B) Pore size distribution analysis of pM-Ru-41-100 (triangle) and pM-Ru-48-50 (circle). (C) The effect of pH on zeta potentials of pM-Ru-41-100 (triangle) and pM-Ru-48-50 (circle).

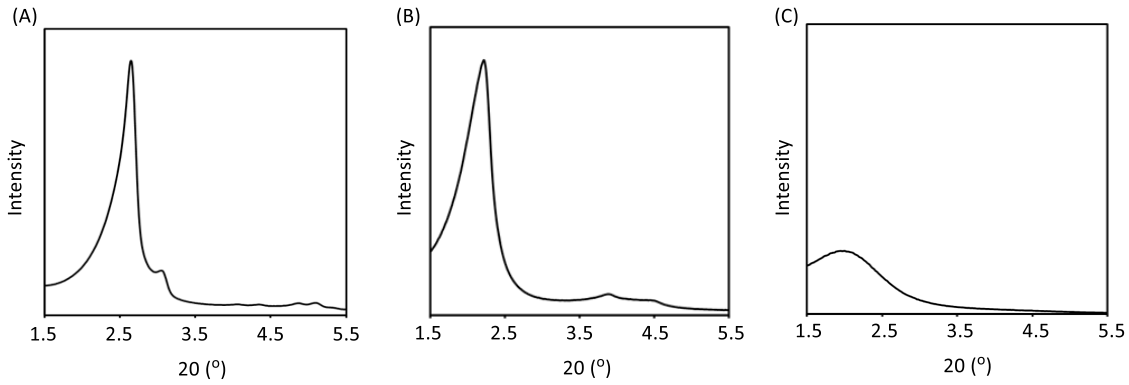

Figure S2. XRD patterns of pM-Ru-48-100 (A), pM-Ru-41-100 (B) and pM-Ru-48-50 (C).

Figure S3. Nanoparticles dispersed in aqueous solution containing sodium phosphate buffer (5 mM, pH 7.0). Left: Nanoparticles with phosphonate groups on their external surface (pM-Ru). Right: Nanoparticles without phosphonate groups on their external surface (M-Ru).

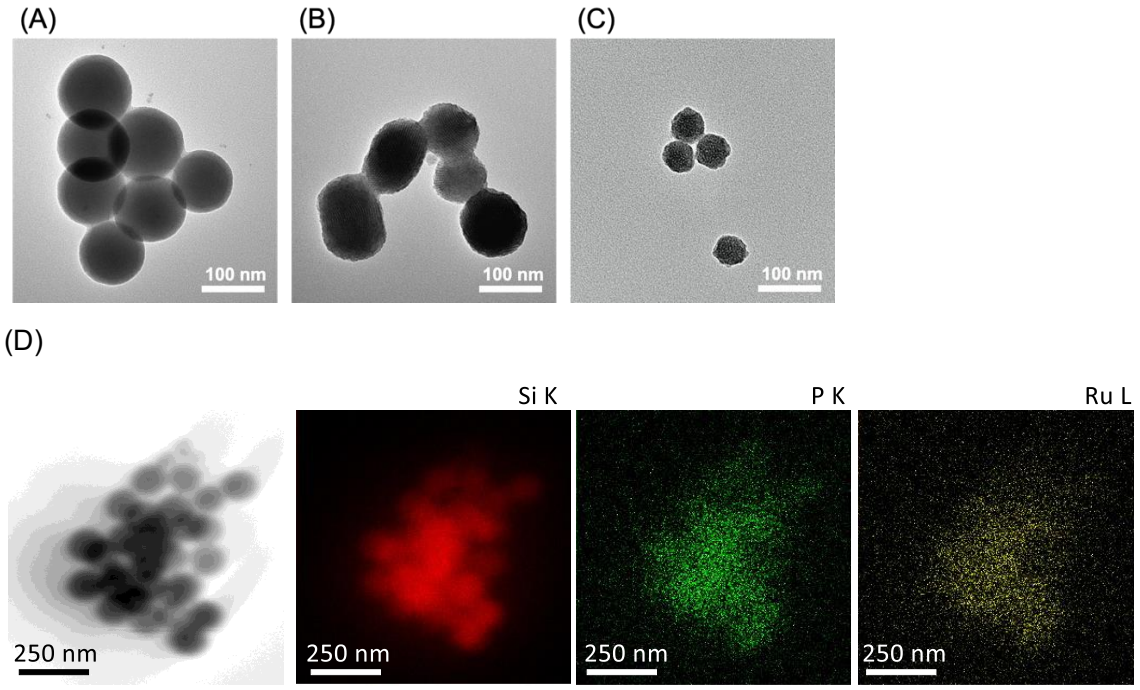

Figure S4. TEM images of (A) pM-Ru-48-100, (B) pM-Ru-41-100 and (C) pM-Ru-48-50. (D) EDX images of pM-Ru-48-100.

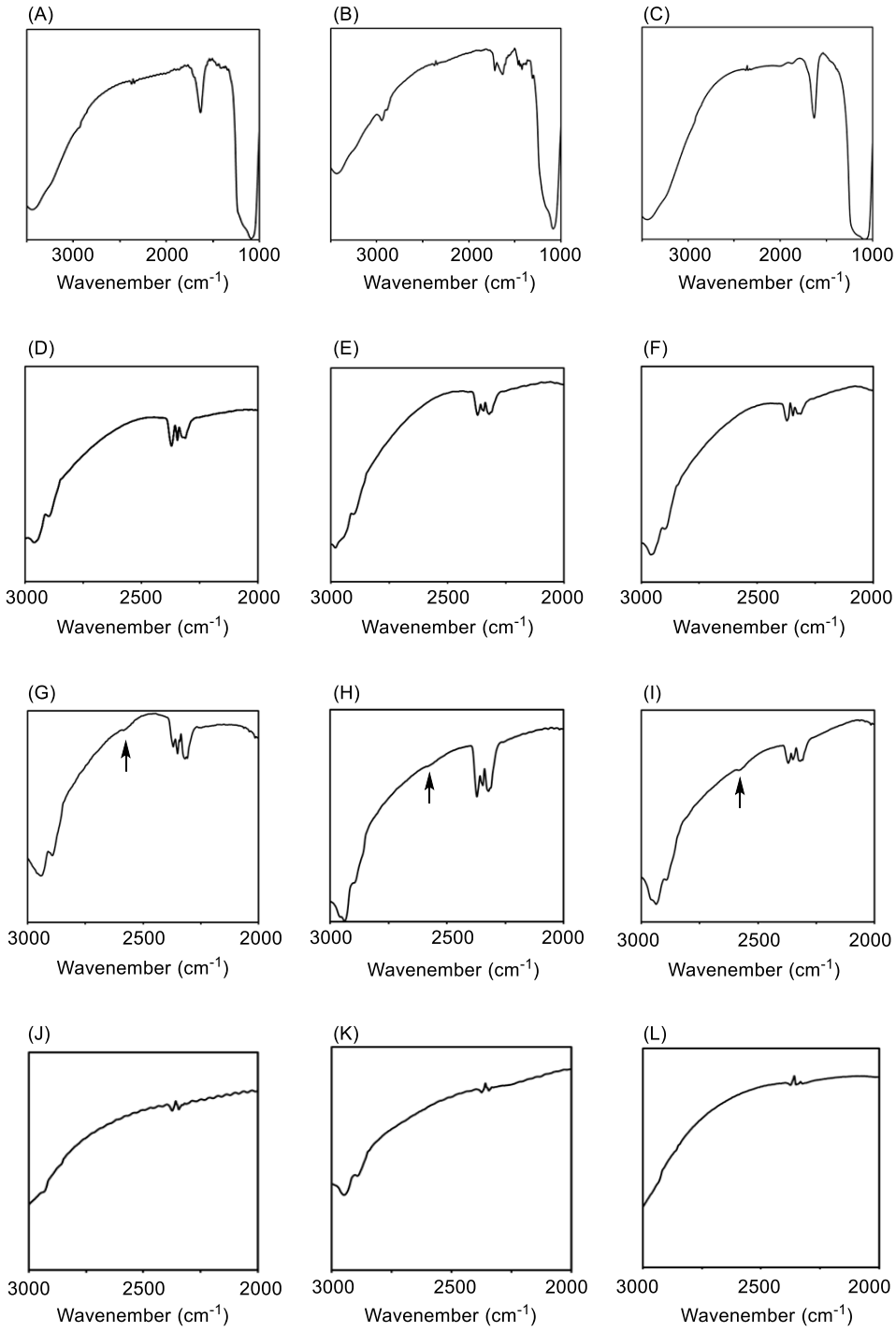

Figure S5. IR spectra of pM-Ru-48-100 (A, D, G, J), pM-Ru-41-100 (B, E, H, K) and pM-Ru-48-50 (C, F, I, L). (A-C) IR spectra (1000-3500 cm^{-1}) of Particle IV. (D-F) Enlarged view of the spectra (2000-3000 cm^{-1}) of Particle II. (G-I) Enlarged view of the spectra (2000-3000 cm^{-1}) of Particle III. Arrows indicate the band (2600 cm^{-1}) attributed to thiol groups. (J-L) Enlarged view of the spectra (2000-3000 cm^{-1}) of Particle IV.

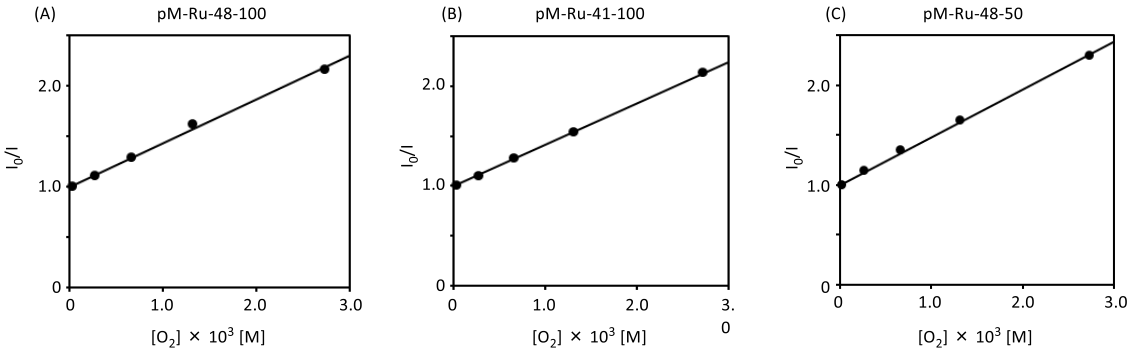

Figure S6. Stern−Volmer plot of the relative phosphorescence intensity (I0/I) of pM-Rus in the presence of oxygen as a quencher. The relative emission intensities of pM-Ru-48-100 (A), pM-Ru-41-100 (B) and pM-Ru-48-50 (C) were plotted against the oxygen concentration.

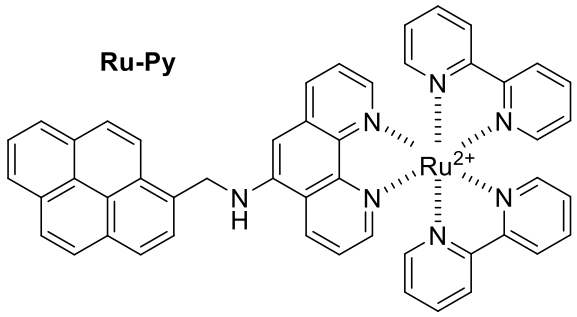

Figure S7. Chemical structure of Ru-Py.

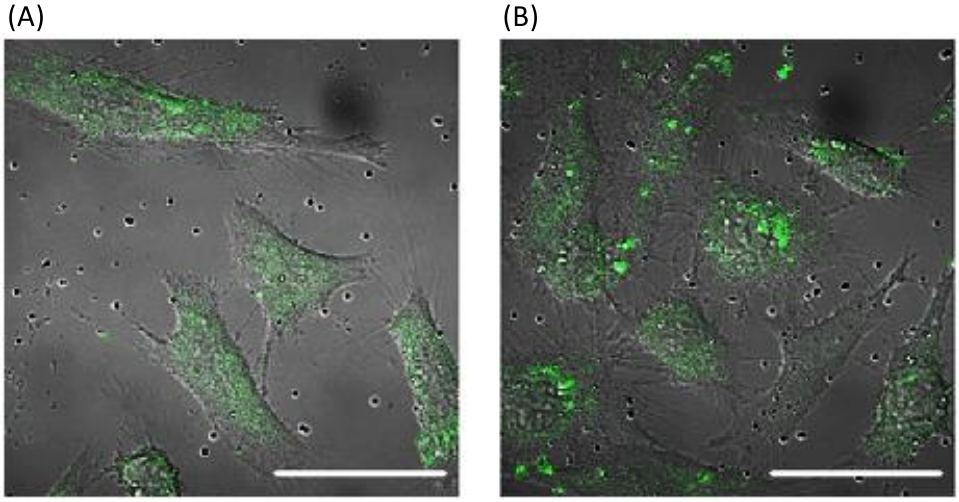

Figure S8. Visualization of singlet oxygen generated in HeLa cells by photoirradiation in the presence of pM-Ru-48-100 (A) and pM-Ru-41-100 (B). Scale bar: 50 μm.