Electronic Supplementary Information

Photodynamic inactivation of *Escherichia coli* by Ru(II) complexes

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Experimental section

The $^1O_2$ quantum yields of the complexes were determined by using $[Ru(bpy)_3]^{2+}$ as the reference (Φ = 0.57 in CH_3CN) and DPBF (1,3-diphenylisobenzofuran) as the trapping agent of $^1O_2$. The n-Octanol/water partition coefficients (log *P*) were determined at 25°C using equal volumes of PBS (2 mL) and 1-octanol (2 mL). The final concentrations of Ru complex in aqueous and organic phases were determined by monitoring the absorbance spectroscopy. UV/Vis absorption spectra were recorded on a Shimadzu UV-1601 spectrophotometer. Emission spectra were run on a Hitachi F-4500 fluorescence spectrophotometer. Fluorescent micrograms were performed on a Nikon C1Si inverted fluorescent microscope and the magnification employed was 10 × 60. The zeta-potentials were measured in PBS suspension on a Malvern Zetasizer 3000HS (Malvern Instruments Ltd.). Transmission electron microscopy (TEM) images were taken by JEOL JEM-2100 LaB6 microscope operated at an accelerating voltage of 200 kV.

A single colony of *E. coli* (JM109) on a solid Luria-Bertani (LB) agar plate was transferred to 8 mL of liquid LB culture medium and was grown at 37 °C for 16 h. Bacteria were harvested by centrifuging at 8000 rpm for 10 min and washing twice

with 5 mM PBS at pH 7.0. The supernatant was discarded and the *E. coli* pellets were resuspended in PBS at a density of 10^8–10^9 cells/mL (absorbance of about 0.7 at 650 nm). The phototoxicity of the Ru(II) complexes were determined by incubation with *E. coli* cell suspensions for 10 min in dark at 37 °C and then exposure to an irradiation of > 450 nm for 5 min (using an Oriel 91192 Solar simulator as light source and a 450 nm cut-off filter to remove the short wavelength light). The treated and control (without Ru(II) complex and without irradiation) bacterial samples were diluted 10^6-fold in PBS. Then the diluted *E. coli* suspension (1 mL) was spread on 3M Petrifilm™ *E. coli* Count Plate and incubated at 37 °C for 48 h. The number of colony-forming units (CFU) was counted by a Shineso G6 Colony Counter. Bacterial killing activity was determined by CFU reduction % (= count of control sample - count of treated sample)/count of control.

The luminescence turn-on of $[Ru(II)(bpy)_2(dppz)]^{2+}$ upon binding to *E. coli*

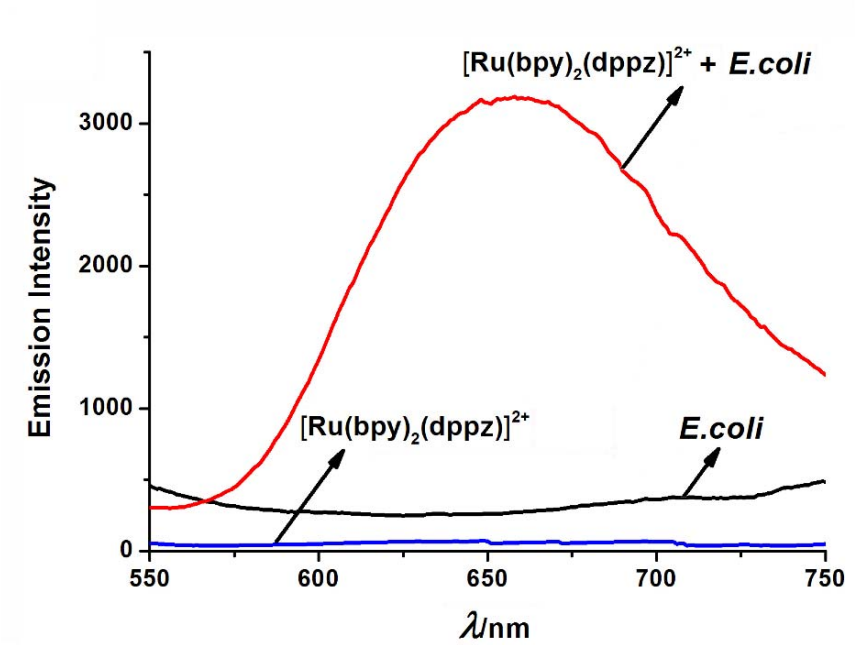

Figure S1. Emission spectra of **2** (10 μM) in PBS in the absence or presence of *E. coli*, excited at 445 nm.

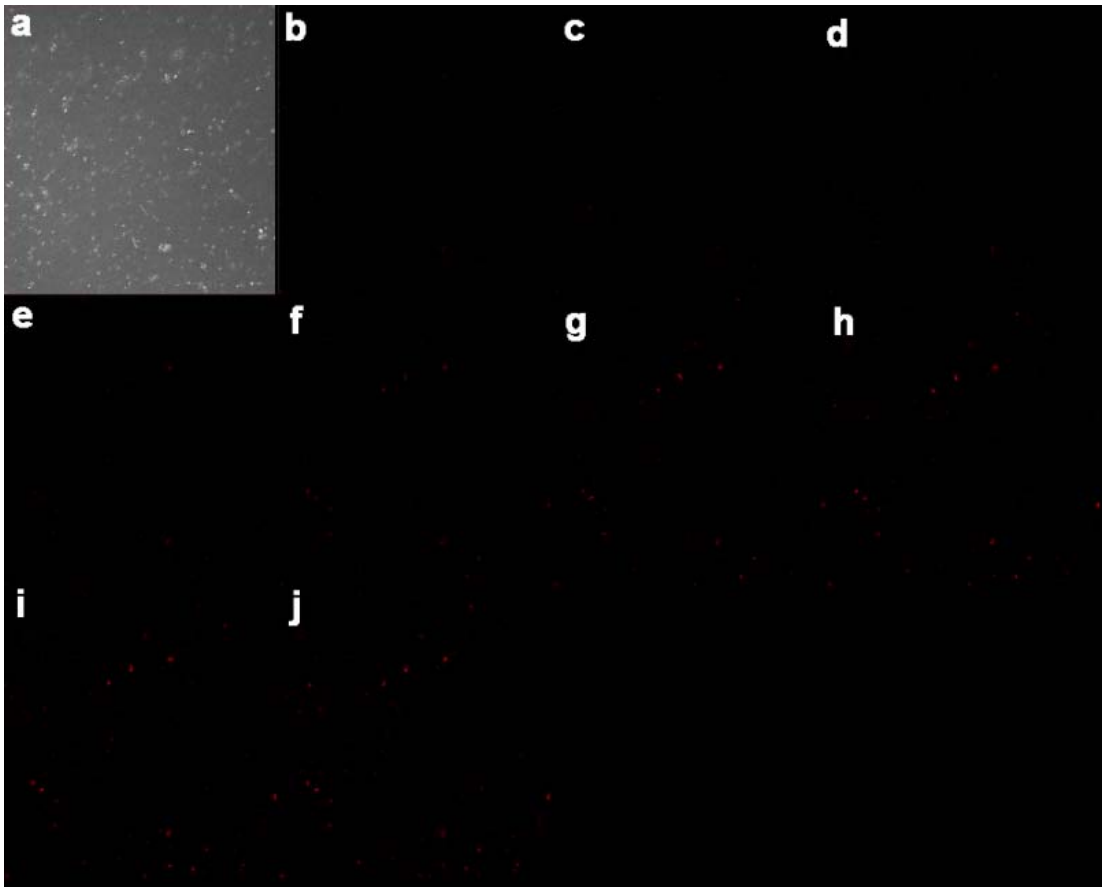

Figure S2. The time-dependent binding of complex **2** to *E. coli* membranes. (a) Bright-field microgram and (b)-(j) fluorescence micrograms of *E. coli* incubated with 5 μM **2** (λ_{ex} = 488 nm), recorded at varied times after addition of **2**: b) 3 min, c) 4 min, d) 5 min, e) 6 min, f) 7 min, g) 8 min, h) 9 min, i) 10 min, j) 40 min.

ζ potential measurements

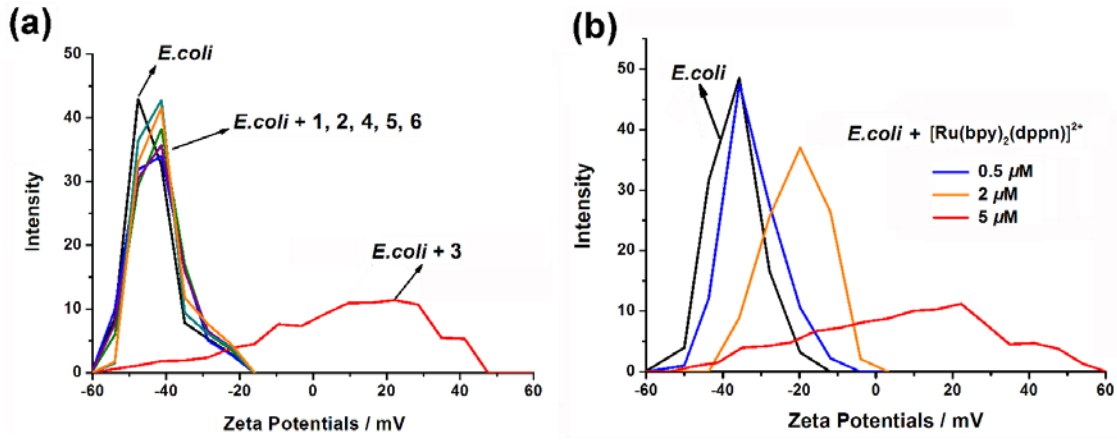

Figure S3. (a) ζ potentials of *E. coli* in PBS buffer solution in the absence or presence of the Ru(II) complexes (5 μM); (b) ζ potentials of *E. coli* in PBS in the presence of varied concentrations of **3**.

Table S1. Zeta potentials of *E.coli* in the absence or presence of the Ru(II) complexes (5 μM).

	E.coli only	*E.coli* + Ru complex					
		1	**2**	**3**	**4**	**5**	**6**
Zeta potential [mV]	-43.2	-42.6	-41.7	+9.2	-42.3	-40.7	-40.5
± [mV]	0.4	0.2	0.4	3.2	0.3	0.3	0.4

Photoinactivation of *E. coli*

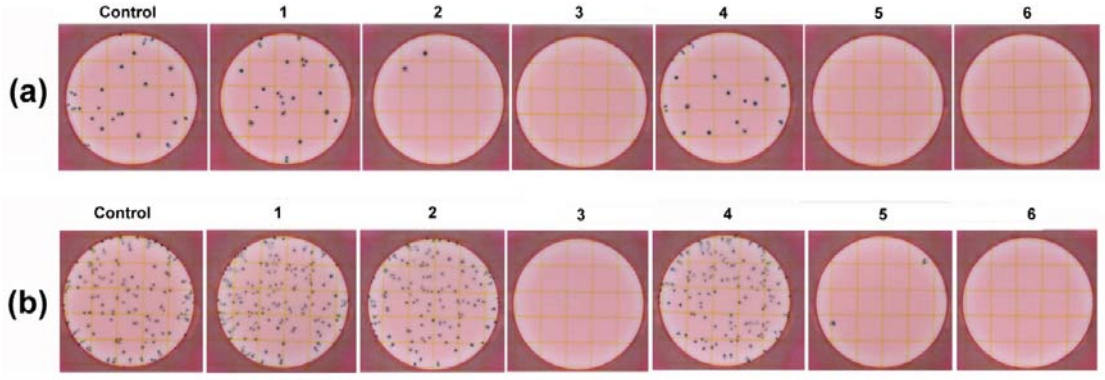

Figure S4. Colony forming units (CFU) of *E. coli* on 3M Petrifilm^{TM} *E.coli* Count Plate. (a) *E. coli* suspensions were incubated with the Ru(II) complexes (2 μM) and then exposed to visible light (> 450 nm) for 5 min; (b) *E. coli* suspensions were incubated with the Ru(II) complexes (2 μM) and then exposed to visible light (> 550 nm) for 10 min. Control experiments were carried out with the cell suspensions irradiated in the absence of the Ru(II) complexes.

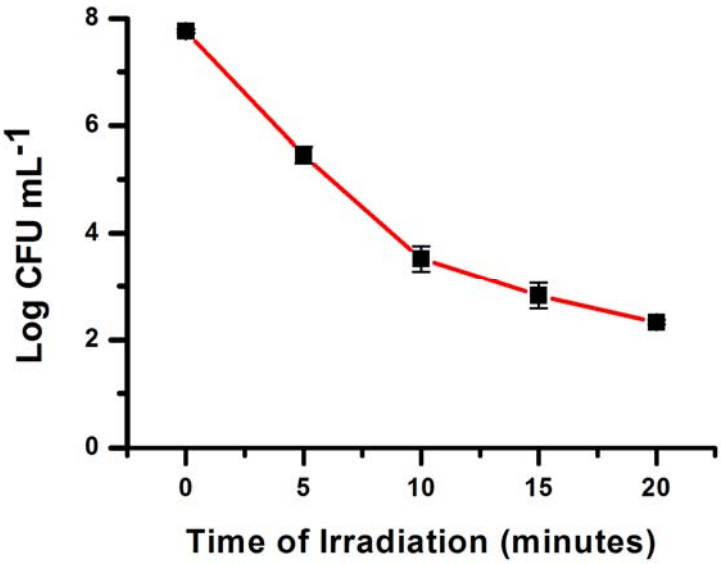

Figure S5. Density variation of *E. coli* in the presence of **3** after irradiation for 5, 10, 15, and 20 min, respectively.

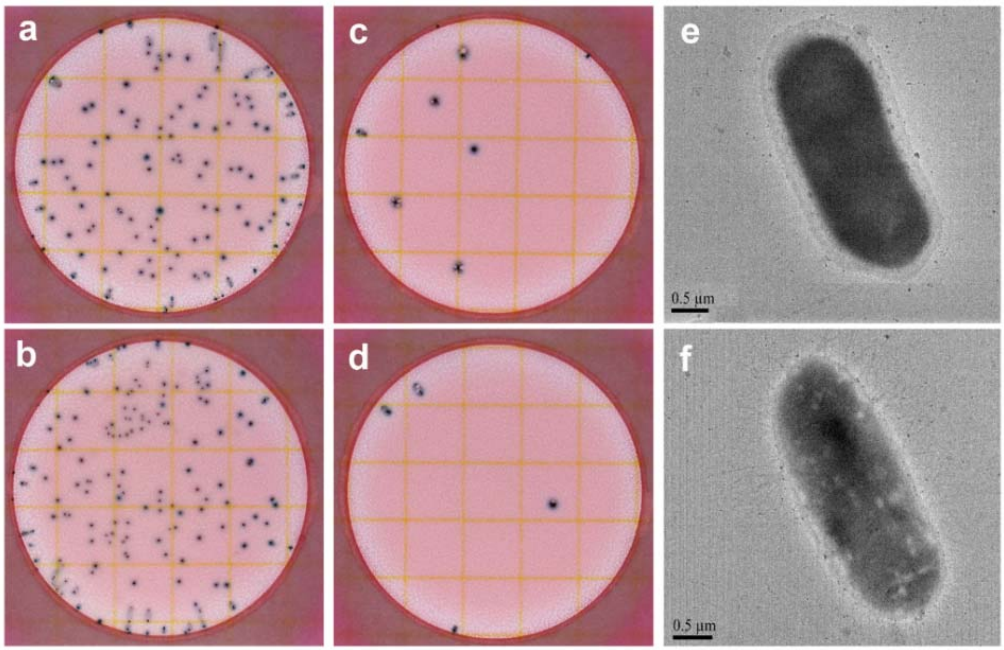

Figure S6. Colony forming units (CFU) of *E. coli* on 3M Petrifilm^{TM} Count Plate and TEM micrographs of *E. coli* thin sections. (a) CFU count without Ru(II) complex in dark; (b) CFU count incubated with **3** (0.5 μM) in dark; (c) CFU count incubated with TMPyP (0.5 μM) and visible irradiation (> 450 nm) for 5 min; (d) CFU count incubated with **3** (0.5 μM) and visible irradiation (>450 nm) for 5 min; (e) TEM micrograph of *E. coli* cell; (f) TEM micrograph of *E. coli* cell treated under the identical condition of (d)

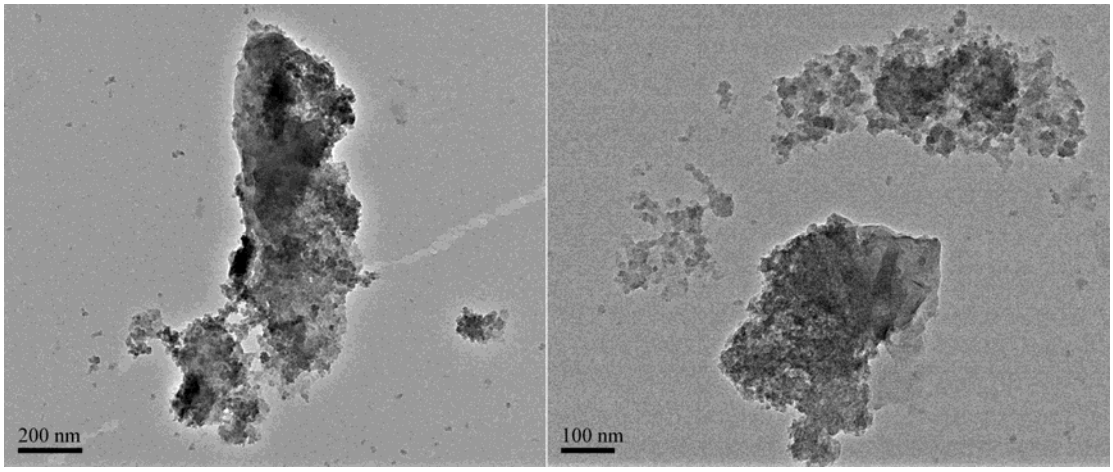

Figure S7. TEM micrographs of the disrupted *E. coli* cells treated with complex **3** (0.5 μM) under visible irradiation (>450 nm) for 5 min.