

*Supplementary information*

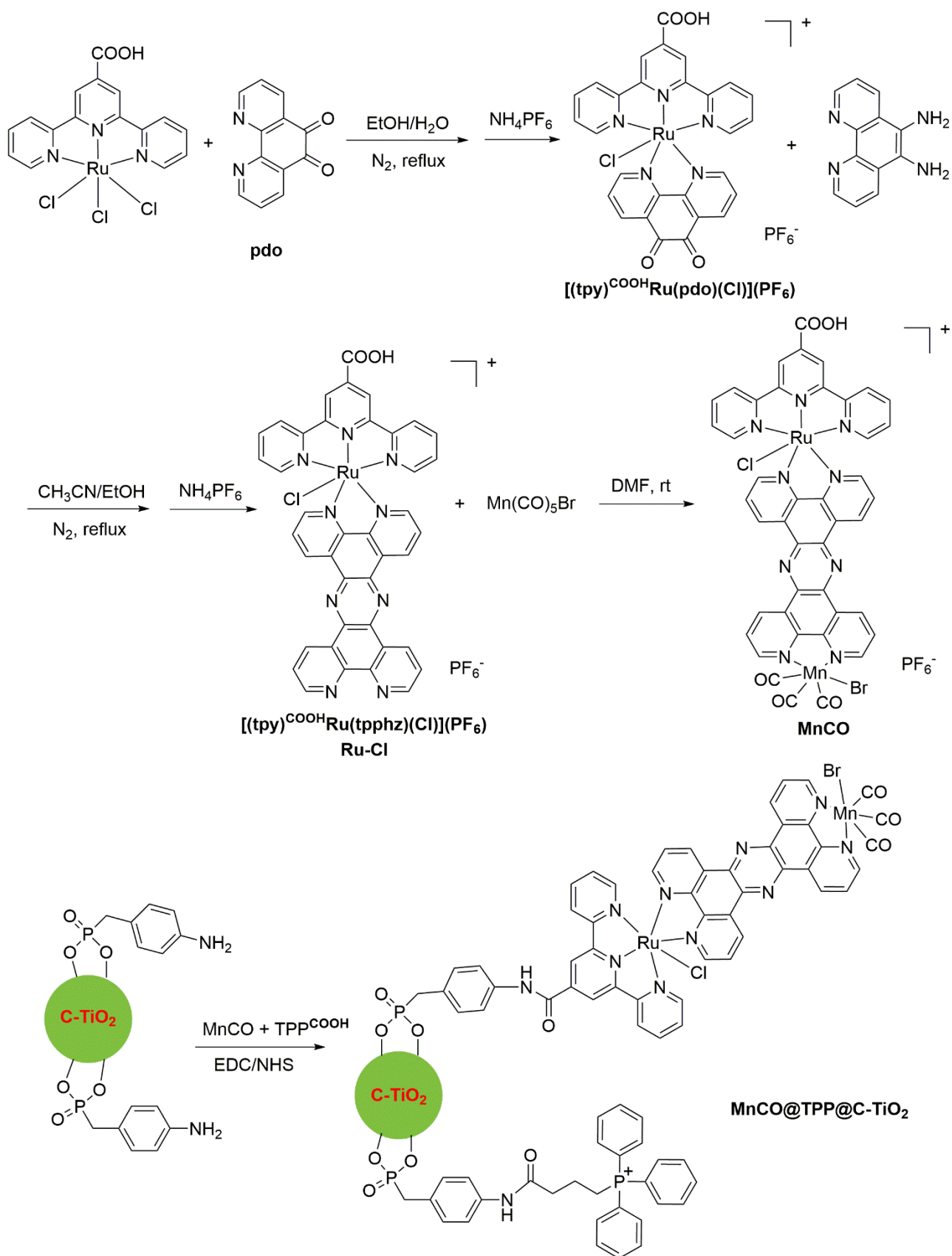
*for:*

**Mitochondria-targeted Carbon Monoxide Delivery Combined with Singlet Oxygen Production from a Single Nanoplatfom under 808 nm Light Irradiation for Synergistic Anticancer Therapy**

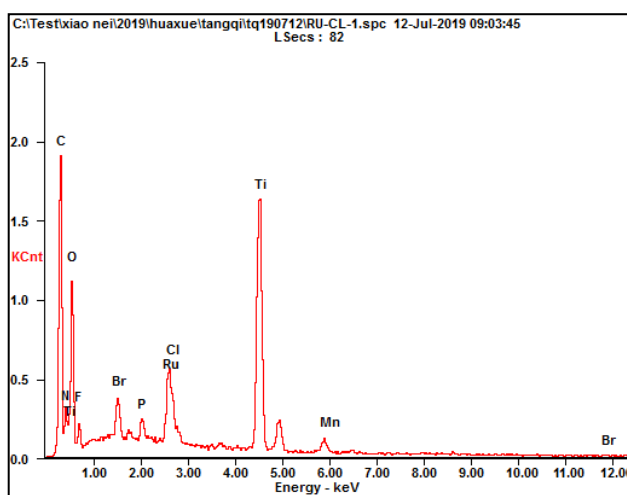
Qi Tang,<sup>†</sup> Hai-Lin Zhang,<sup>†</sup> Yi Wang,<sup>†</sup> Jing Liu,<sup>†</sup> Shi-Ping Yang,<sup>§</sup> and Jin-Gang Liu<sup>\*,†</sup>

<sup>†</sup>Key Laboratory for Advanced Materials, School of Chemistry & Molecular Engineering, East China University of Science and Technology, Shanghai 200237, P. R. China, E-mail: liujingang@ecust.edu.cn

<sup>§</sup>Key Lab of Resource Chemistry of MOE & Shanghai Key Lab of Rare Earth Functional Materials, Shanghai Normal University, Shanghai 200234, P. R. China



**Scheme S1** Preparation procedures of nanoplatform (1).



<i>Element</i>	<i>Wt %</i>	<i>At %</i>
<i>CK</i>	28.61	50.82
<i>NK</i>	00.18	00.27
<i>OK</i>	19.63	26.17
<i>FK</i>	02.20	02.48
<i>BrL</i>	03.03	00.81
<i>PK</i>	00.85	00.59
<i>RuL</i>	06.63	01.40
<i>ClK</i>	02.27	01.36
<i>TiK</i>	33.17	14.77
<i>MnK</i>	03.43	01.33

Fig. S1 EDS spectrum of nanoplateform (1).

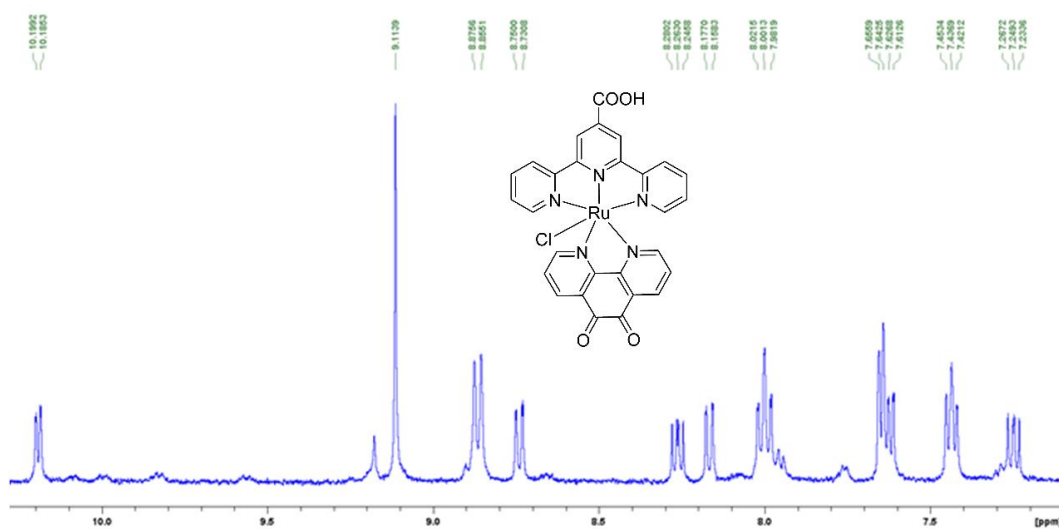
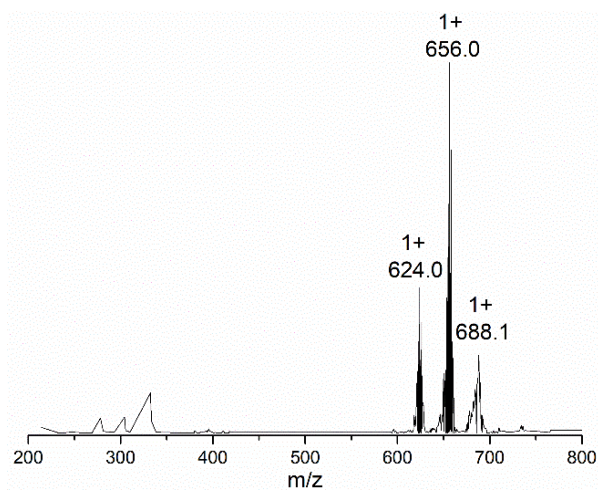
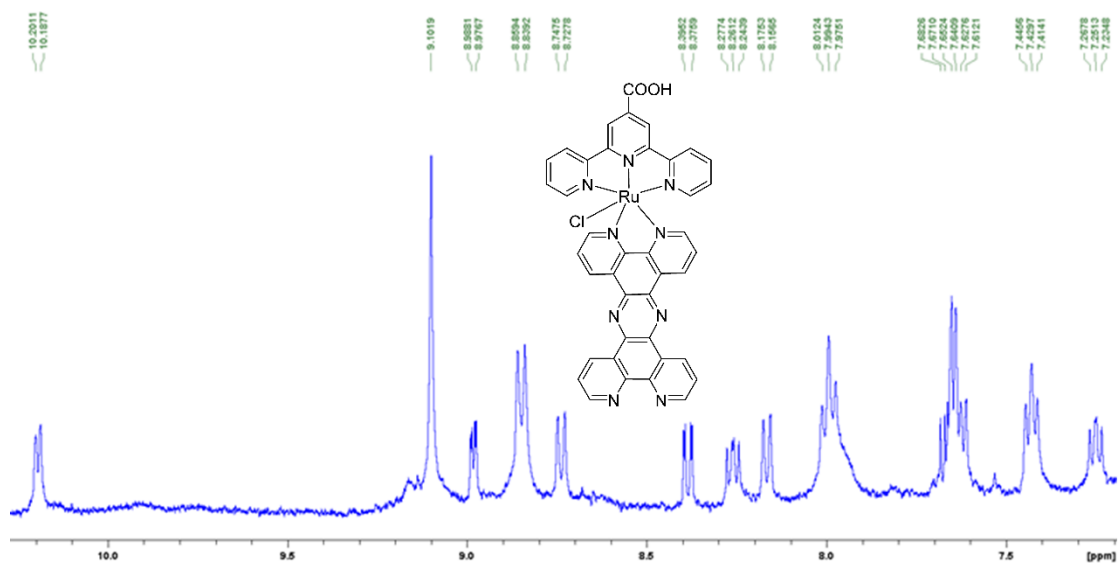


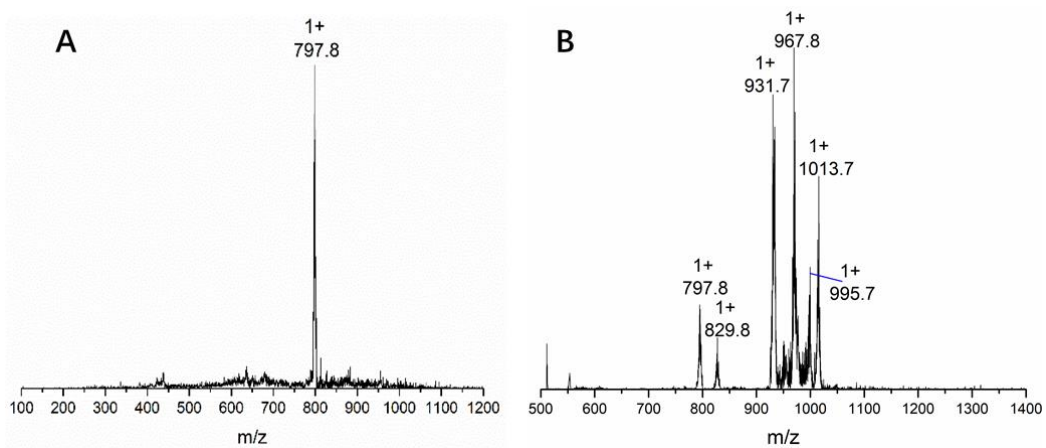
Fig. S2 <sup>1</sup>H NMR spectrum of [(tpy<sup>COOH</sup>)Ru(pdo)(Cl)](PF<sub>6</sub>) in DMSO-*d*<sub>6</sub>.



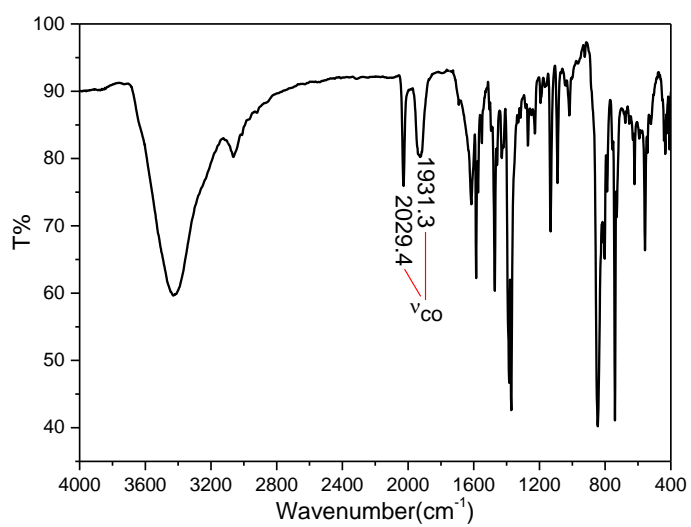
**Fig. S3** ESI Mass spectrum of  $[(\text{tpy}^{\text{COOH}})\text{Ru}(\text{pdo})(\text{Cl})](\text{PF}_6)$ .



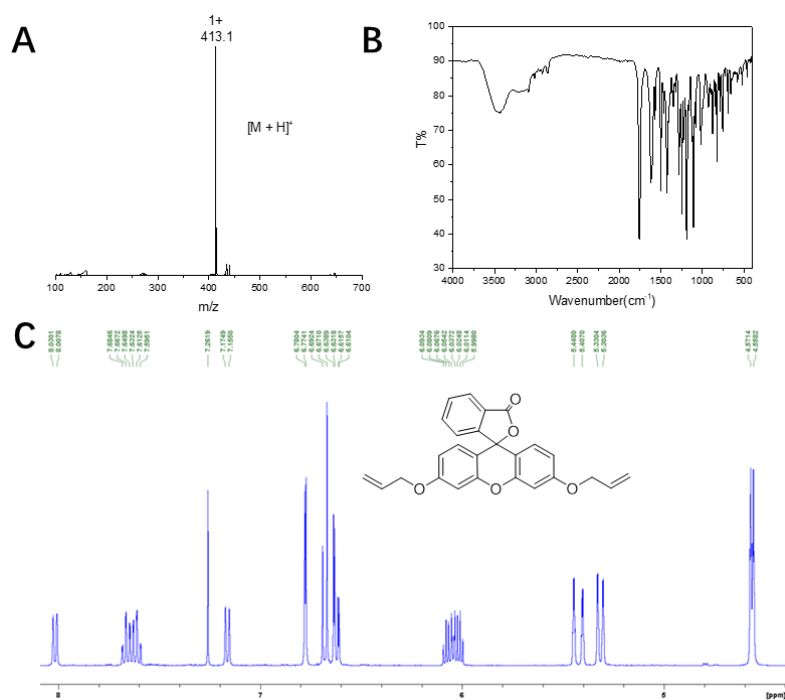
**Fig. S4**  $^1\text{H}$  NMR spectrum of  $[(\text{tpy}^{\text{COOH}})\text{Ru}(\text{tpphz})(\text{Cl})](\text{PF}_6)$  in  $\text{DMSO-}d_6$ .



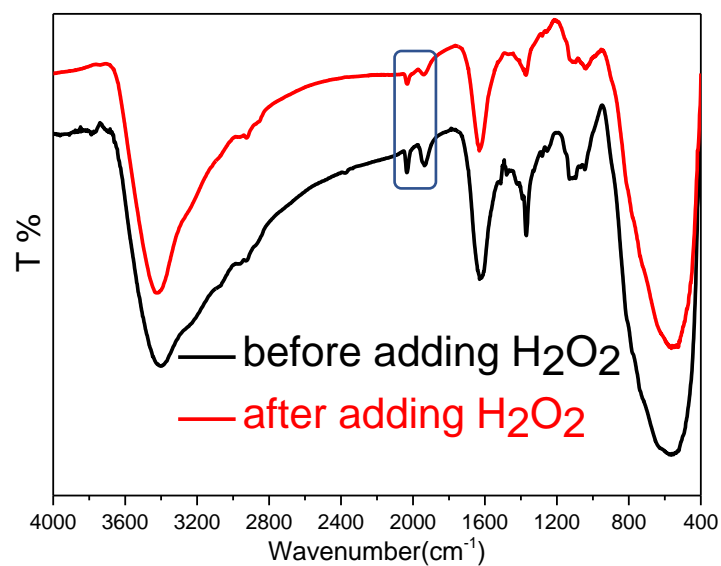
**Fig. S5** ESI Mass spectra of  $[(\text{tpy}^{\text{COOH}})\text{Ru}(\text{tpphz})(\text{Cl})](\text{PF}_6)$  (A) and Mn-CO (B).



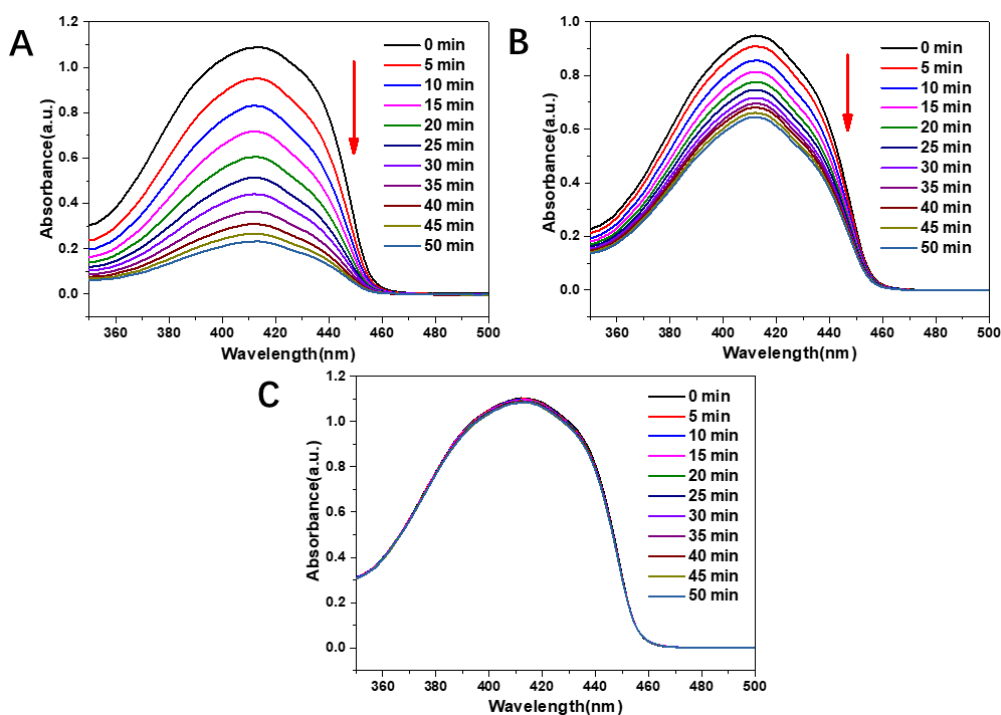
**Fig. S6** FTIR spectrum of Mn-CO.



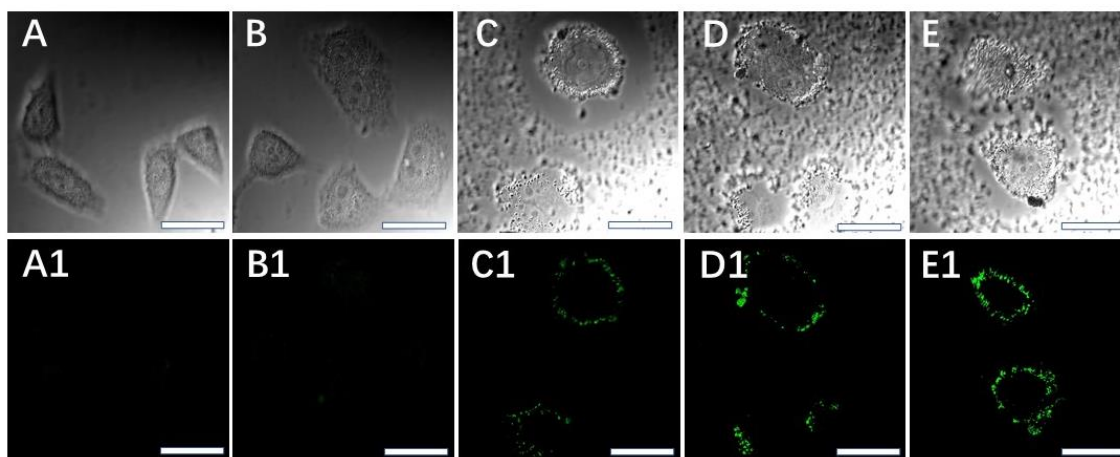
**Fig. S7** ESI Mass spectrum (A), FTIR spectrum (B) and  $^1\text{H}$  NMR spectrum (C) of the CO probe (FL-CO-1).



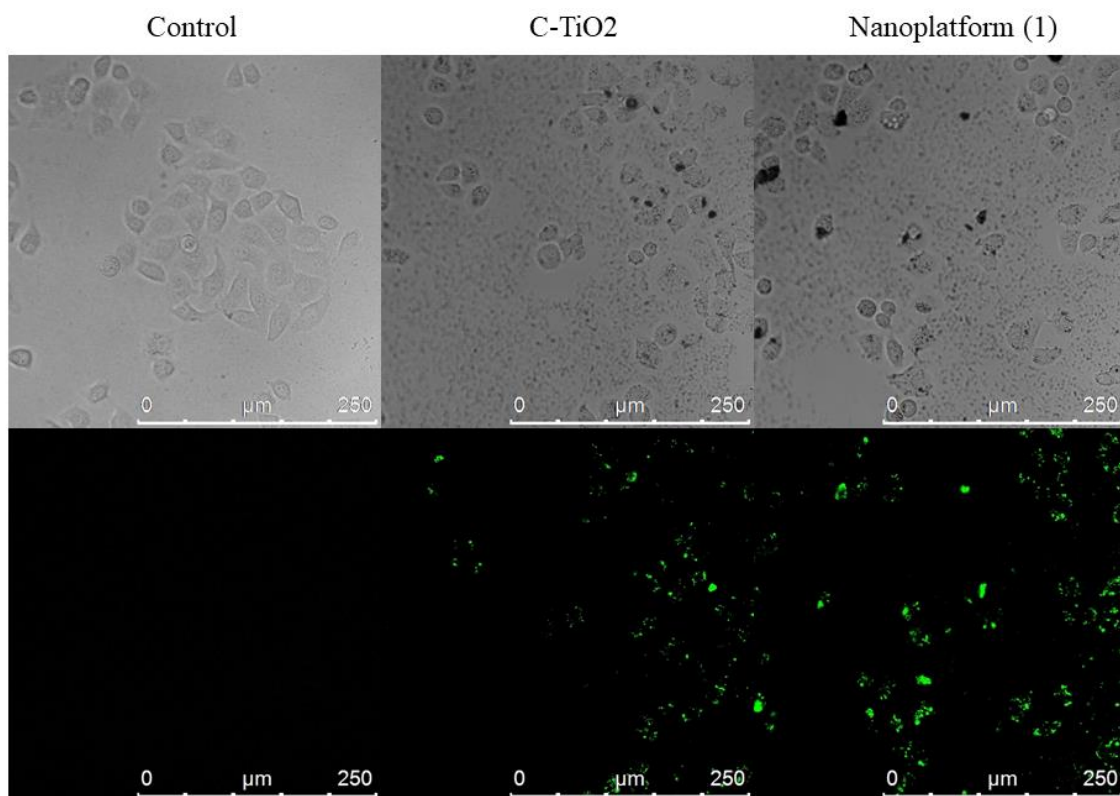
**Fig. S8** FTIR spectrum of nanoplatform (1) before and after adding  $100 \mu\text{M}$   $\text{H}_2\text{O}_2$ .



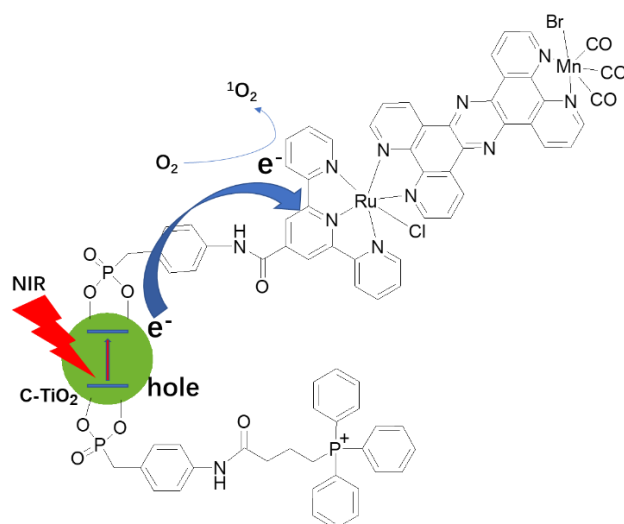
**Fig. S9** Absorbance spectrum changes of DPBF treated with nanoplatform (1) (A) and C-TiO<sub>2</sub> (B) after 808 nm laser (1.0 W/cm<sup>2</sup>) irradiation for different times. (C) Absorbance spectrum changes of DPBF treated with 808 nm laser (1.0 W/cm<sup>2</sup>) only.



**Fig. S10** Intracellular fluorescence image of CO by probe system (probe + PdCl<sub>2</sub>, 1 μM each). Top row A-E: bright field image. Bottom row: fluorescence images of A-E, respectively. (A, A1) The HeLa cells were incubated with probe for 30 min. (B, B1) The HeLa cells were incubated with PdCl<sub>2</sub> for 30 min. (C and C1, D and D1, E and E1) The HeLa cells were preincubated with 50, 100 and 200 μM of nanoplatform (1) for 4 h and then incubated with probe and PdCl<sub>2</sub> for 30 min, respectively. Scale bars: 25 μm.



**Fig. S11** Intracellular fluorescence image of  $^1\text{O}_2$  by DCFH-DA. Top row: bright field image. Bottom row: fluorescence images. Scale bars: 250  $\mu\text{m}$ .



**Fig. S12** Plausible mechanism for  $^1\text{O}_2$  production by nanoplatfrom (1).