**Supporting Information**

# Cyclometalated iridium(III) complexes with imidazo[4,5-f][1,10]phenanthroline derivatives for mitochondrial imaging in living cells

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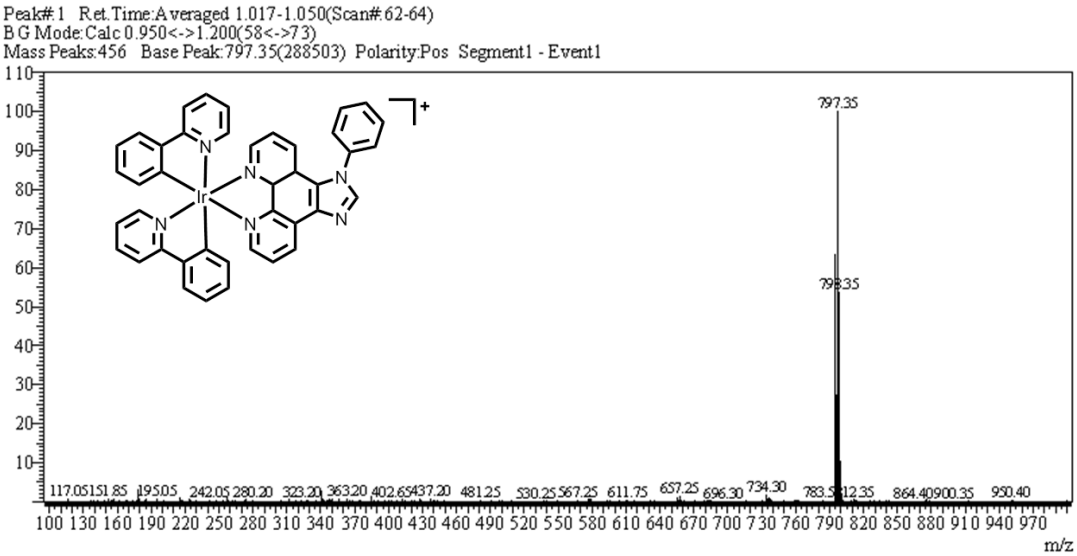


**Fig. S1** ES-MS spectra of **MitoIr1** in $CH_3OH$ solutions.

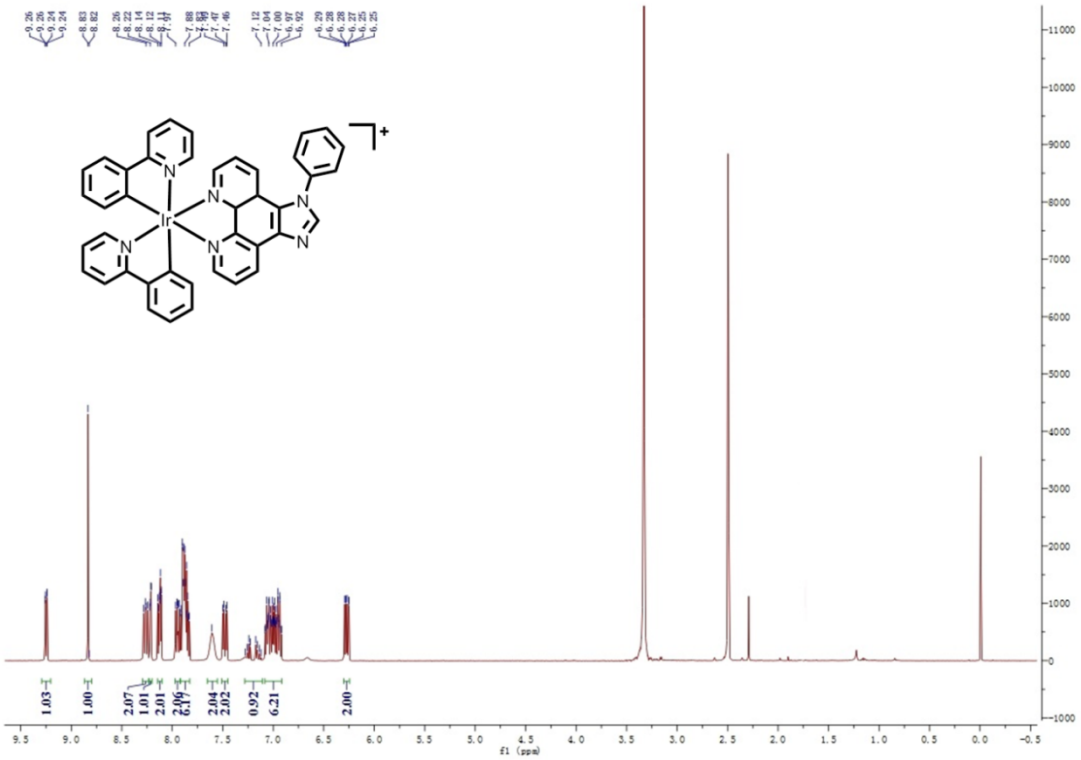


**Fig. S2** $^1$HNMR spectra of **MitoIr1** in DMSO-$d_6$, 500 MHz.

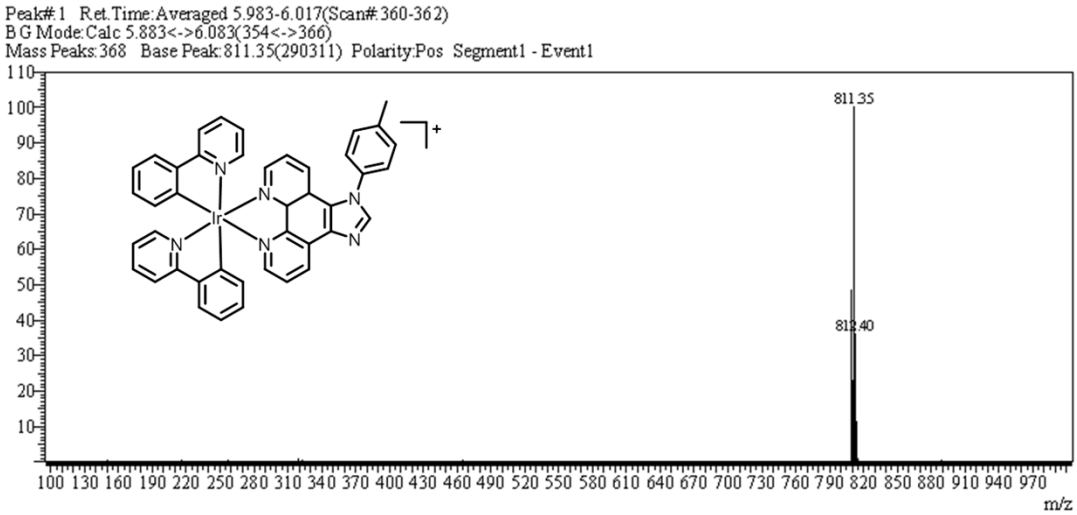


**Fig. S3** ES-MS spectra of**MitoIr2** in $CH_3OH$ solutions.

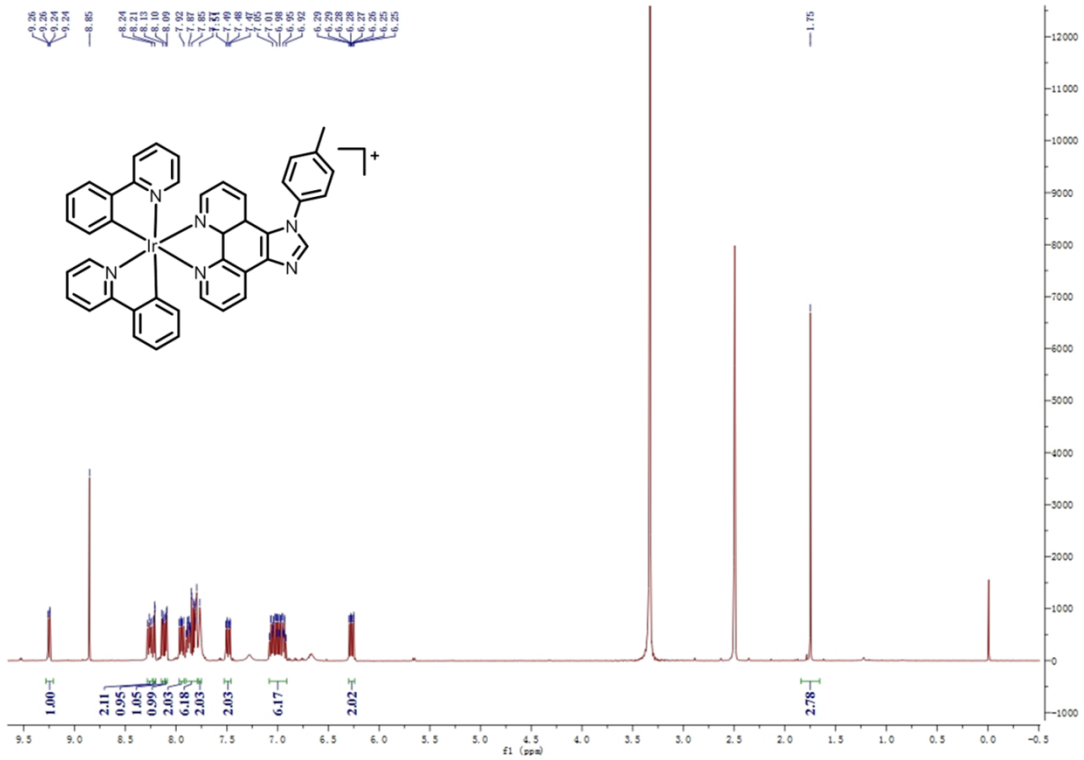


**Fig. S4** $^1$HNMR spectra of **MitoIr2** in DMSO-$d_6$, 500 MHz.

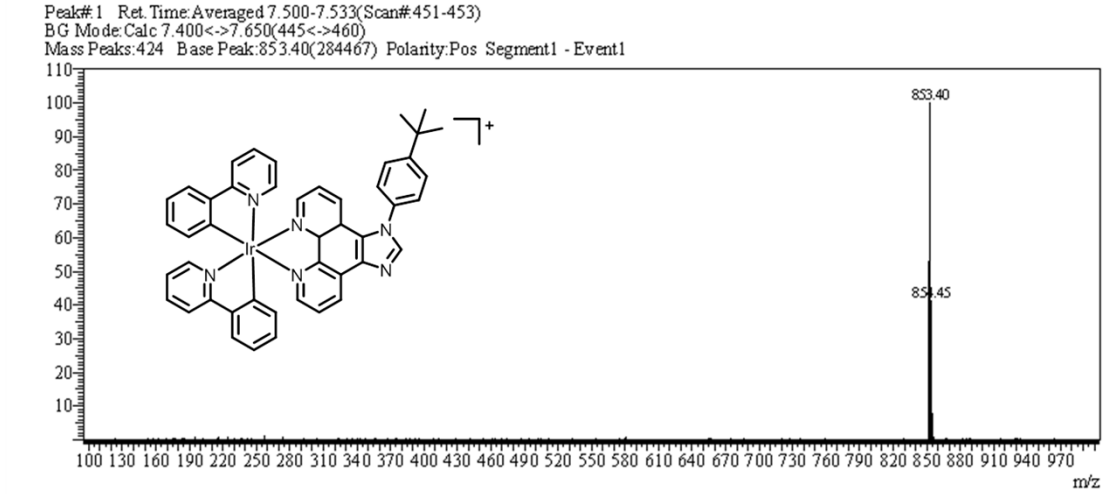


**Fig. S5** ES-MS spectra of **MitoIr3** in $CH_3OH$ solutions.

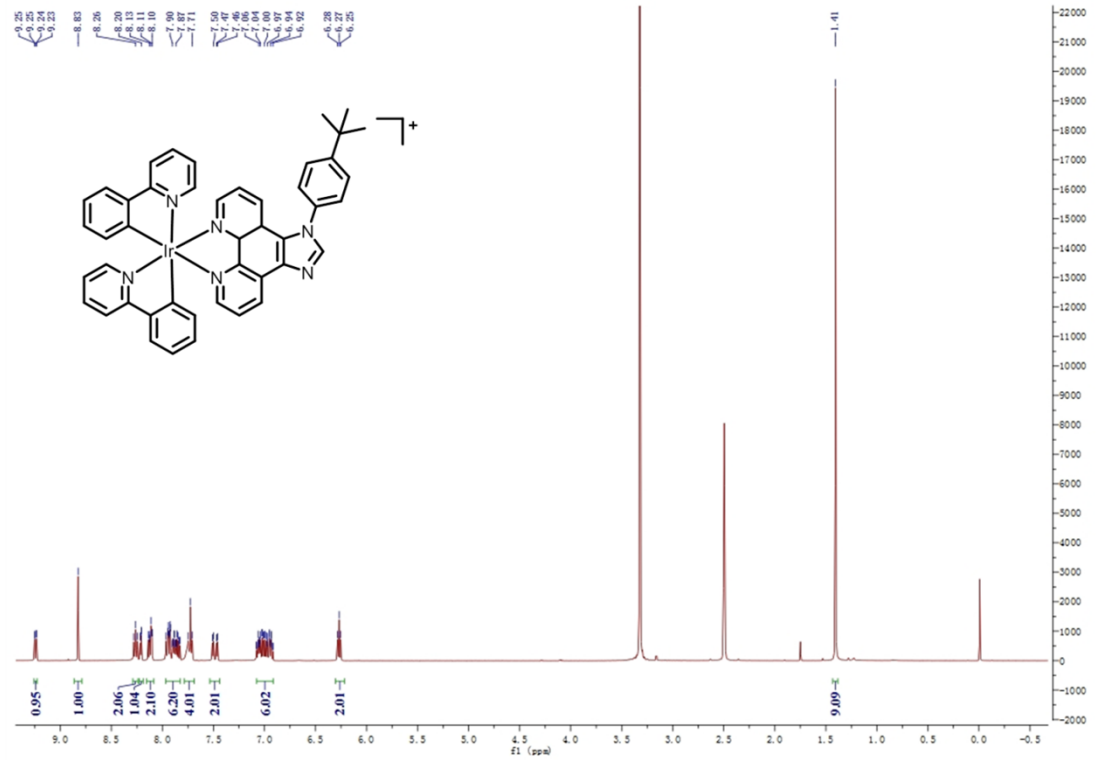


**Fig. S6** $^1$HNMR spectra of **MitoIr3** in DMSO-$d_6$, 500 MHz.

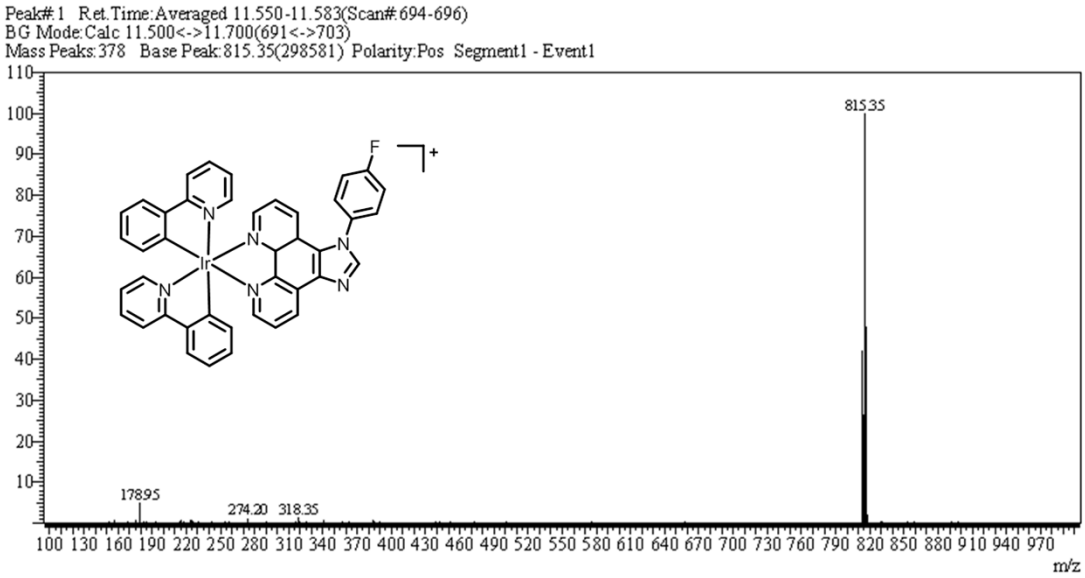


**Fig. S7** ES-MS spectra of **MitoIr4** in $CH_3OH$ solutions.

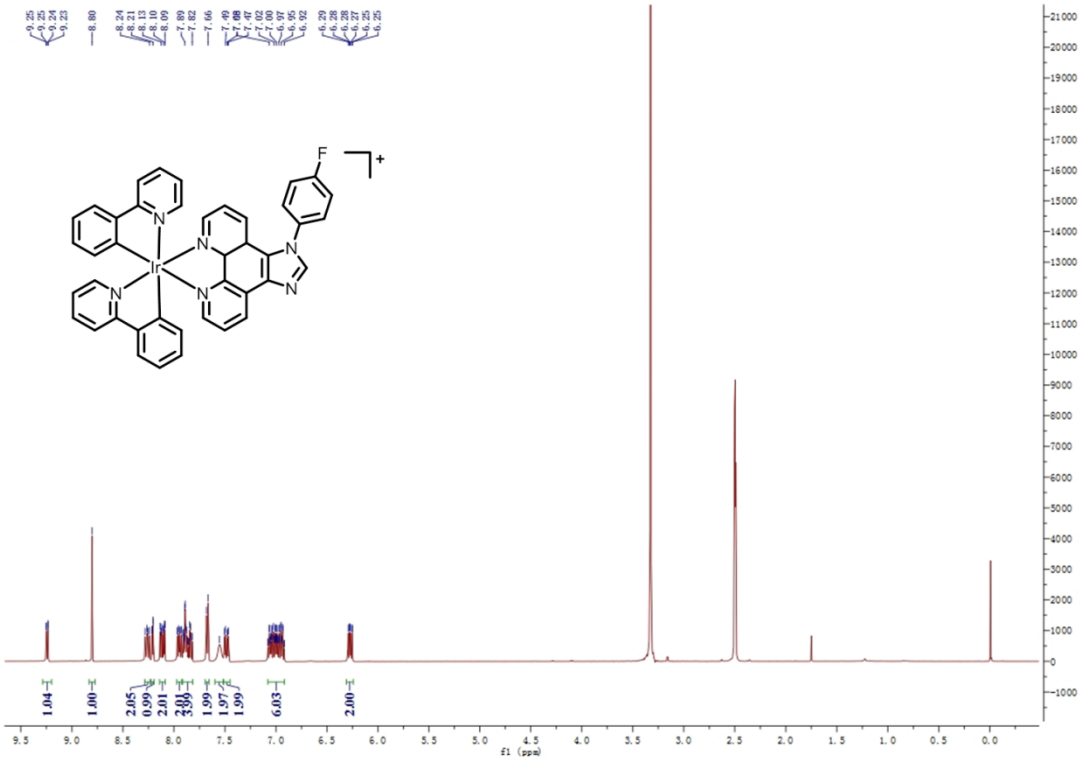

**Fig. S8** $^1$HNMR spectra of **MitoIr4** in DMSO-$d_6$, 500 MHz.

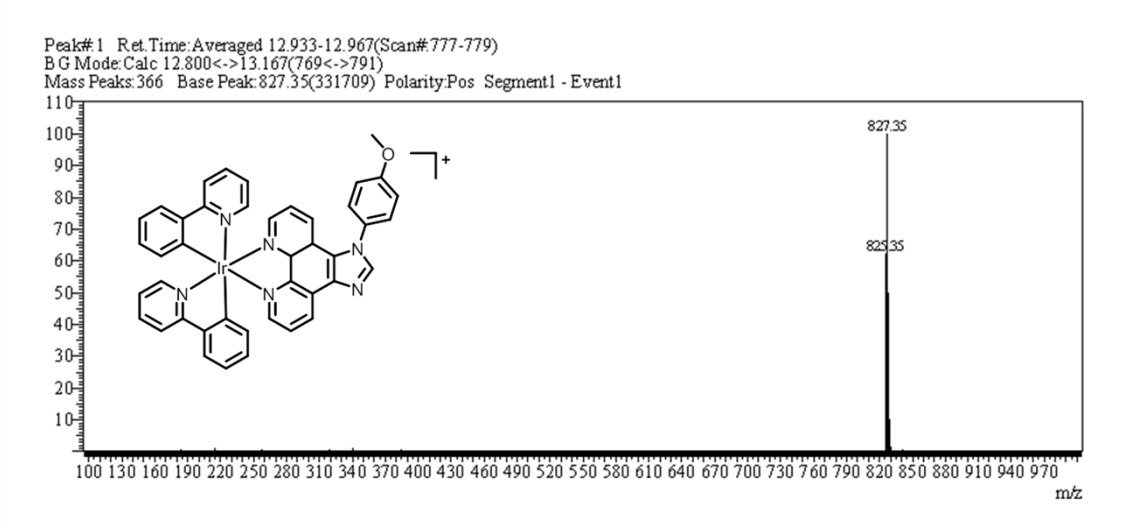


**Fig. S9** ES-MS spectra of **MitoIr5** in $CH_3OH$ solutions.

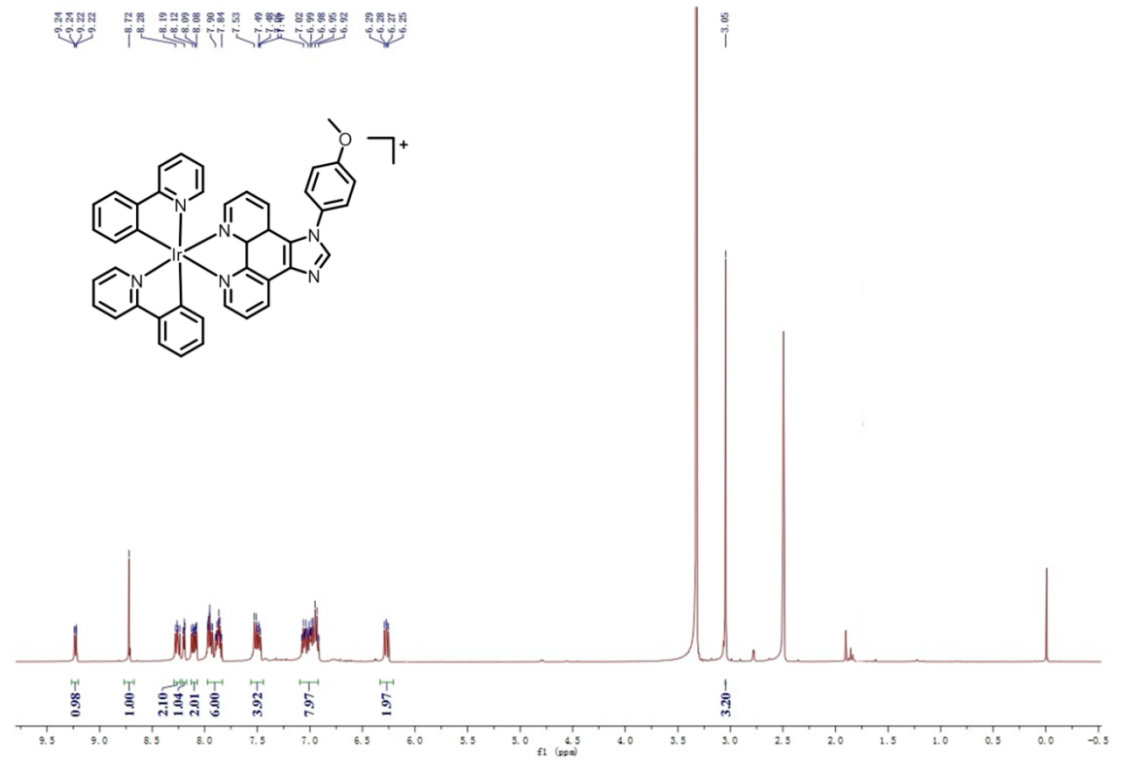

**Fig. S10** $^1$HNMR spectra of **MitoIr5** in in DMSO-$d_6$, 500 MHz.

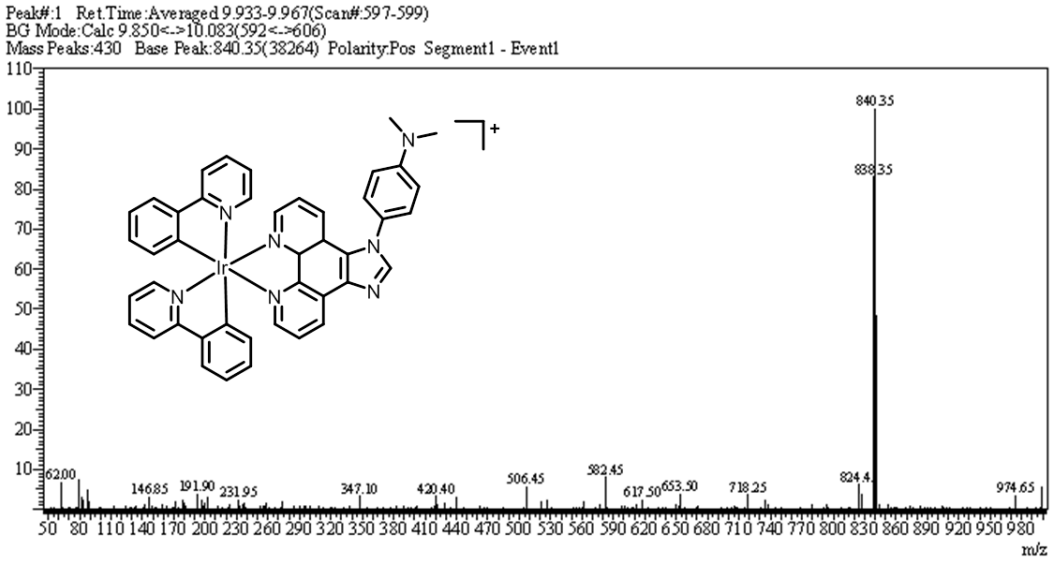


**Fig. S11** ES-MS spectra of **MitoIr6** in $CH_3OH$ solutions.

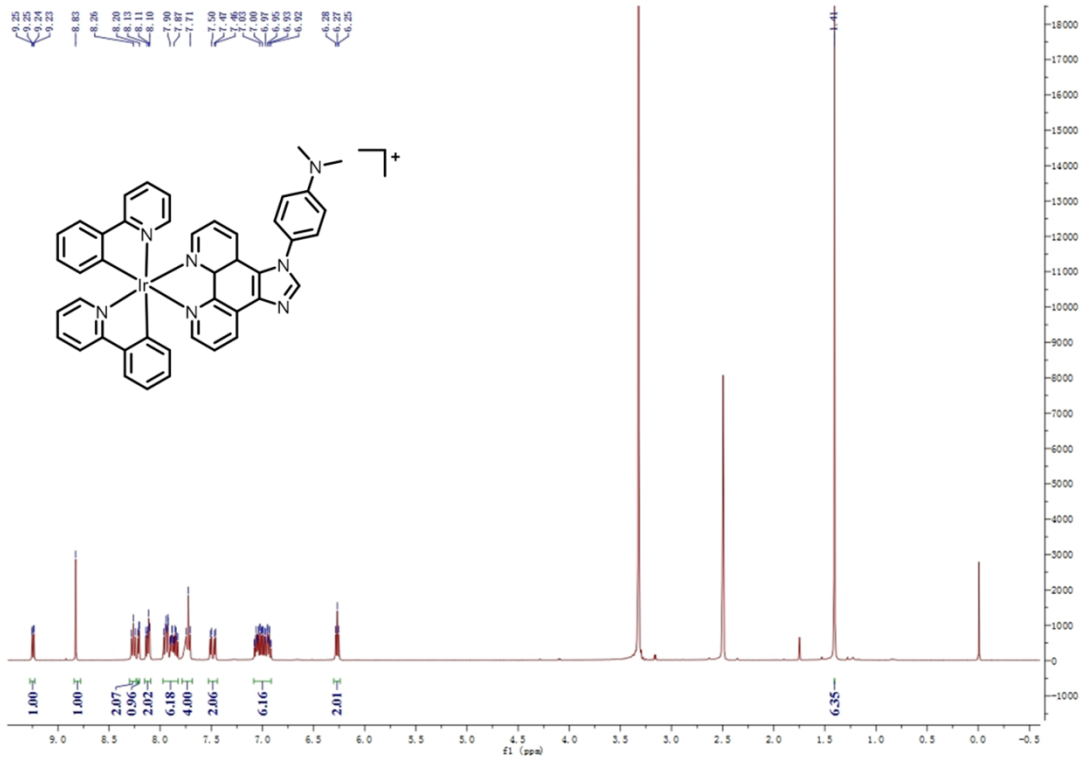

**Fig. S12** $^1$HNMR spectra of **MitoIr6** in DMSO-$d_6$, 500 MHz.

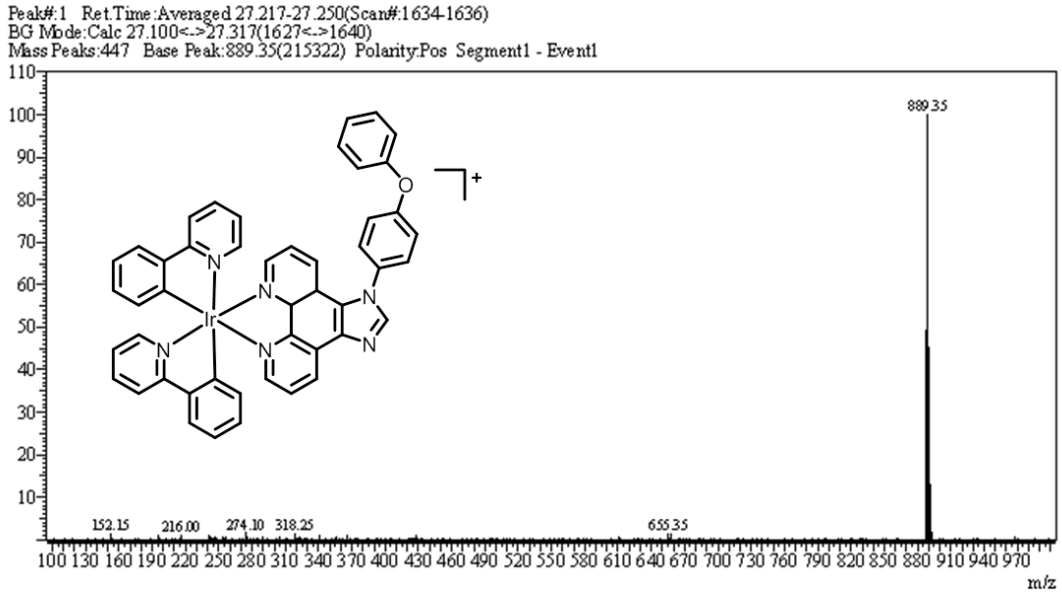


**Fig. S13** ESI-MS spectra of **MitoIr7** in $CH_3OH$ solutions.

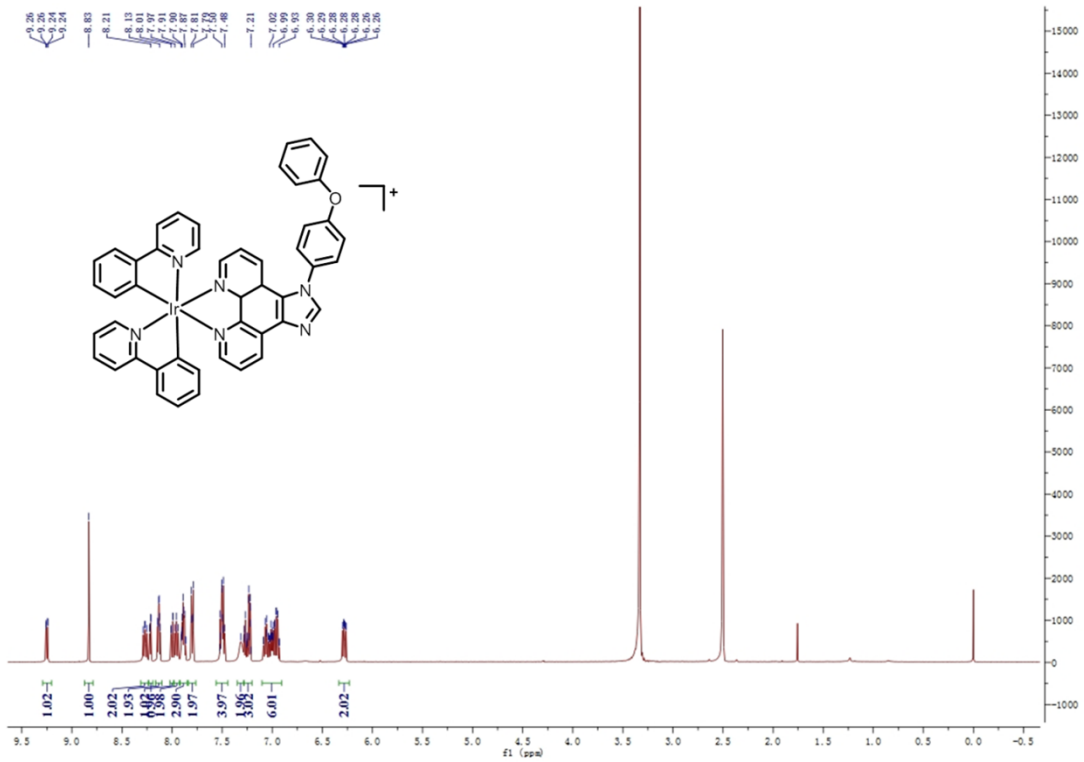

**Fig. S14** $^1$HNMR spectra of **MitoIr7** in DMSO-$d_6$, 500 MHz.

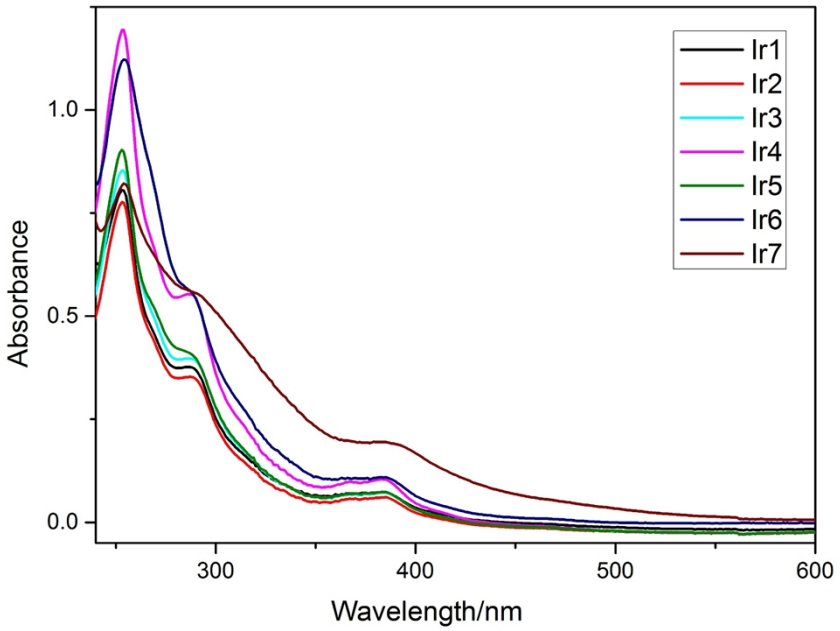


**Fig. S15** Absorption spectra of **MitoIr1-MitoIr7** (10 μM) in a DMSO/PBS (v/v = 1:999) solution at 298K.

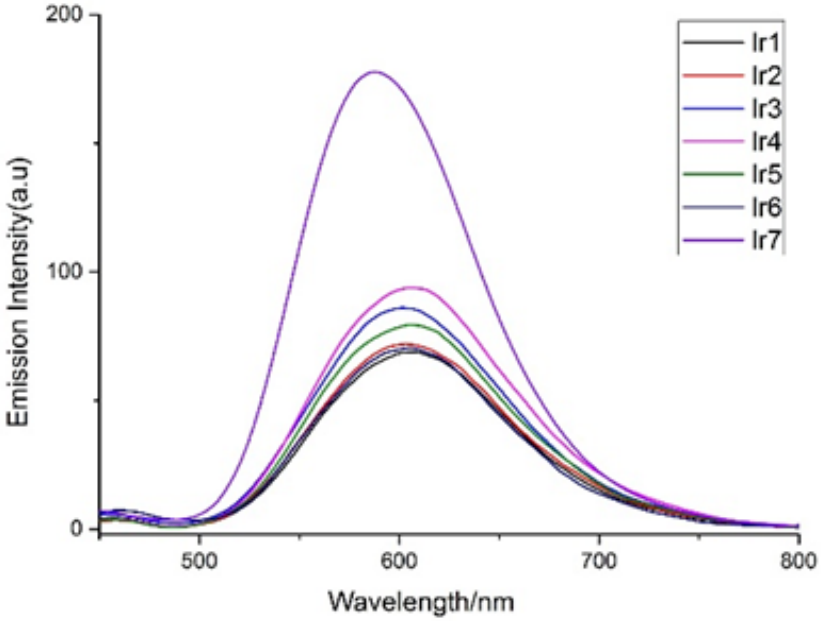


**Fig. S16** Emission spectra of **MitoIr1-MitoIr6** (10 μM) and **MitoIr7** (2 μM) in a DMSO/PBS (v/v = 1:999) solution at 298K with an excitation wavelength of 384 nm.

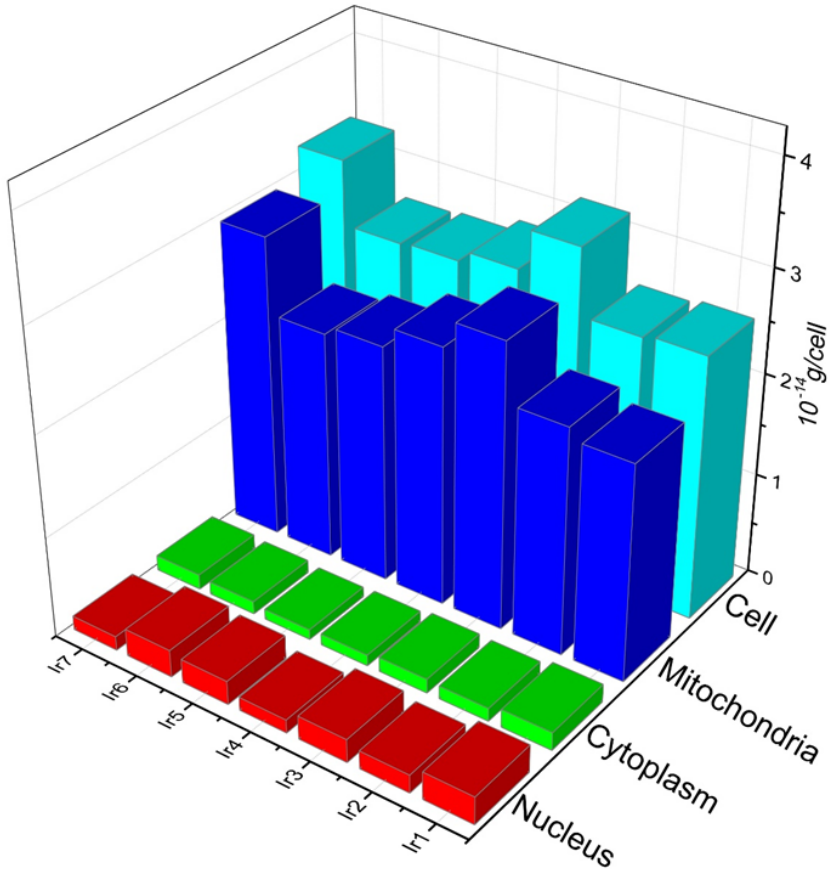


**Fig. S17** Distribution analysis of **MitoIr1–MitoIr7** in HeLa cells by ICP-MS.

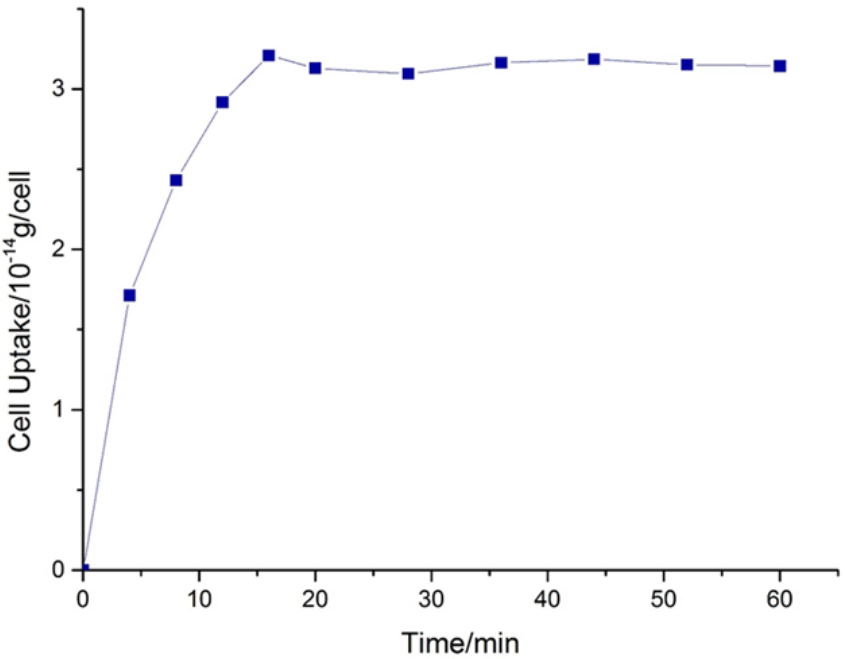


**Fig. S18** Time-dependent cell uptake of **MitoIr7** by ICP-MS.

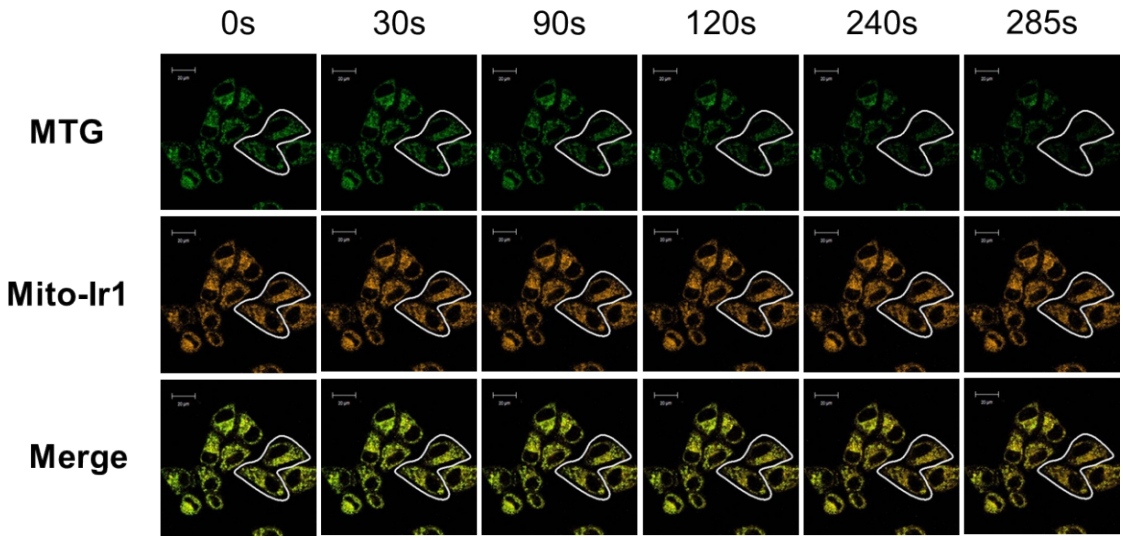


**Fig. S19** Photobleaching experiments of **MitoIr1** in HeLa cells.

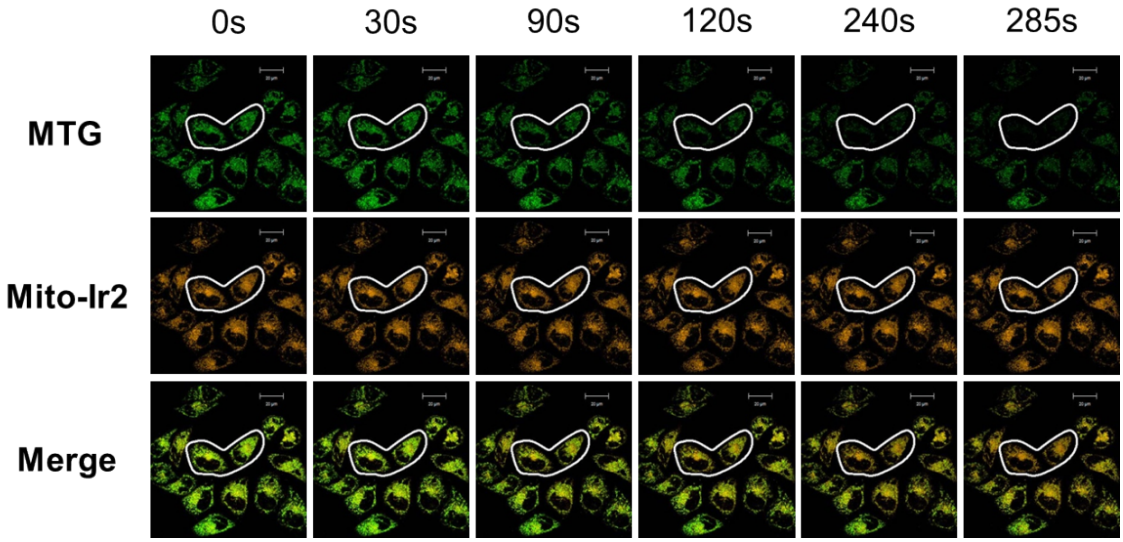


**Fig. S20** Photobleaching experiments of **MitoIr2** in HeLa cells.

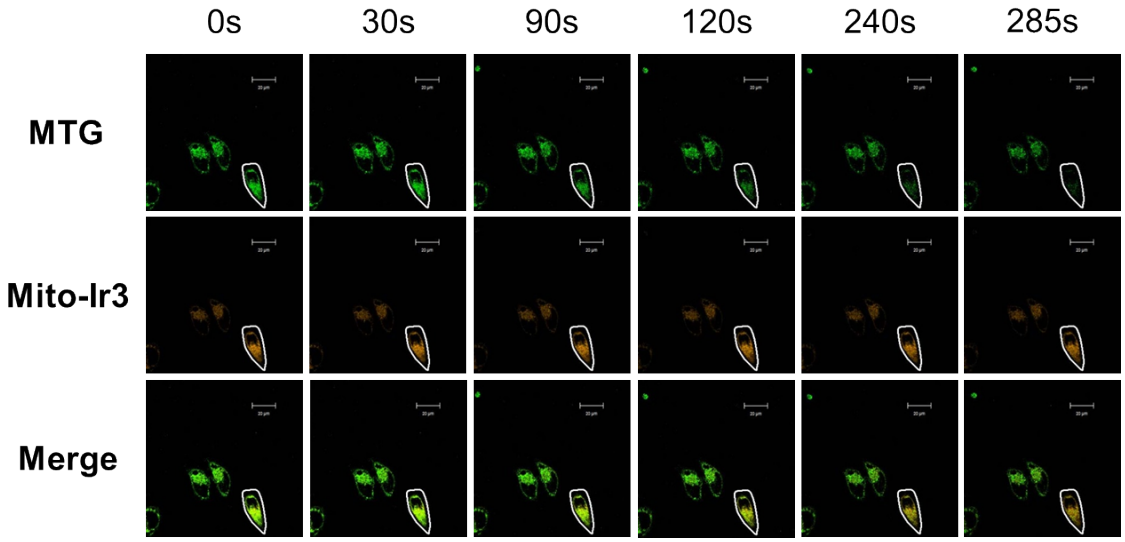


**Fig. S21** Photobleaching experiments of **MitoIr3** in HeLa cells.

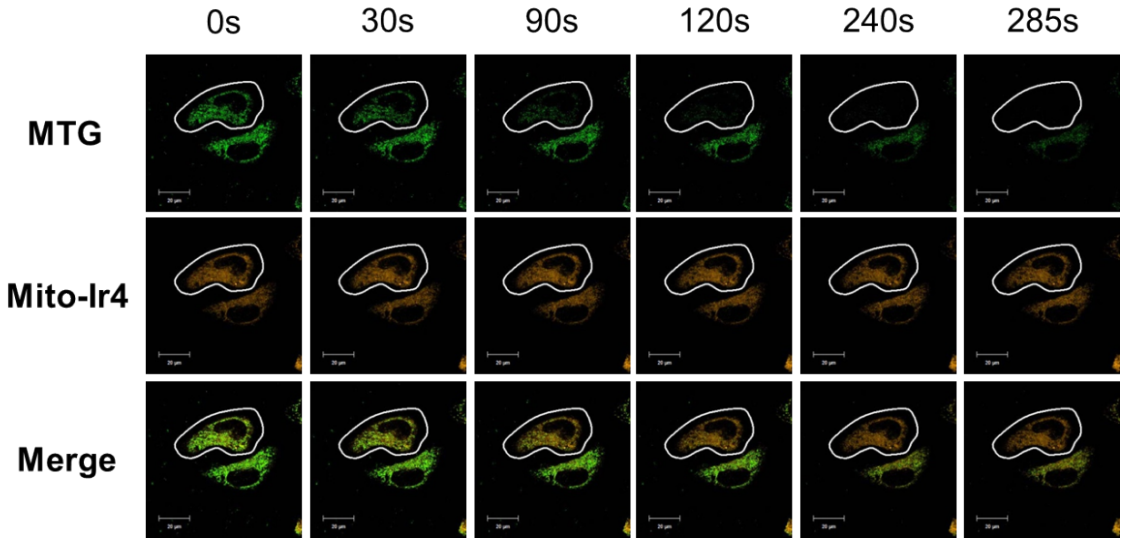


**Fig. S22** Photobleaching experiments of **MitoIr4** in HeLa cells.

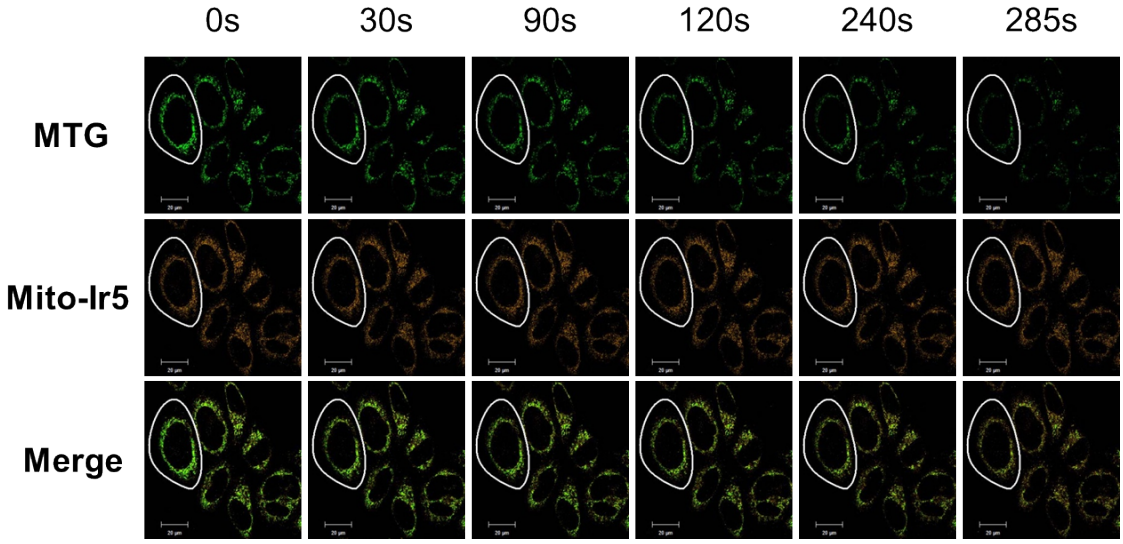


**Fig. S23** Photobleaching experiments of **MitoIr5** in HeLa cells.

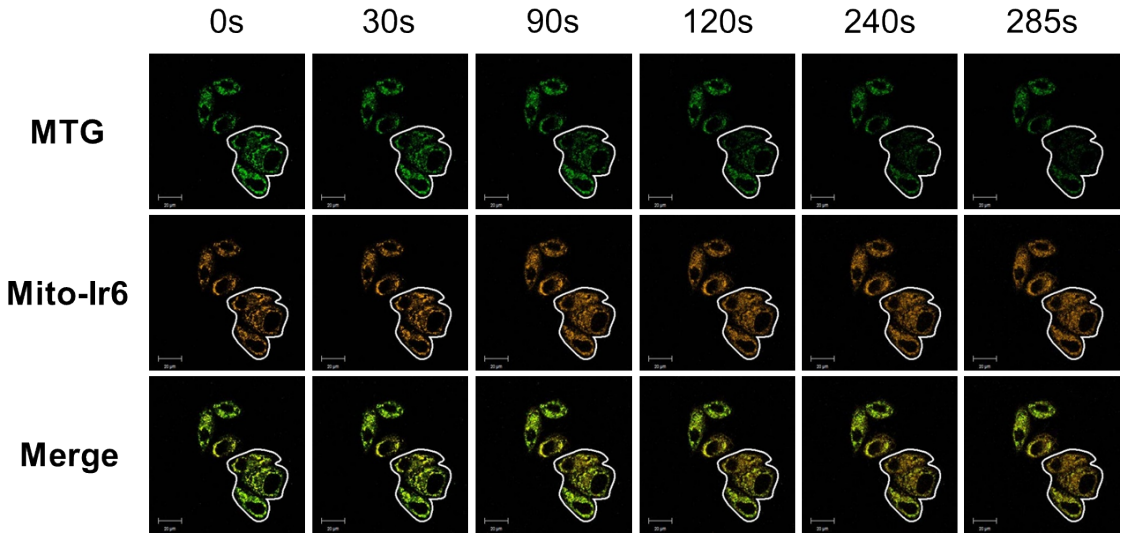


**Fig. S24** Photobleaching experiments of **MitoIr6** in HeLa cells.

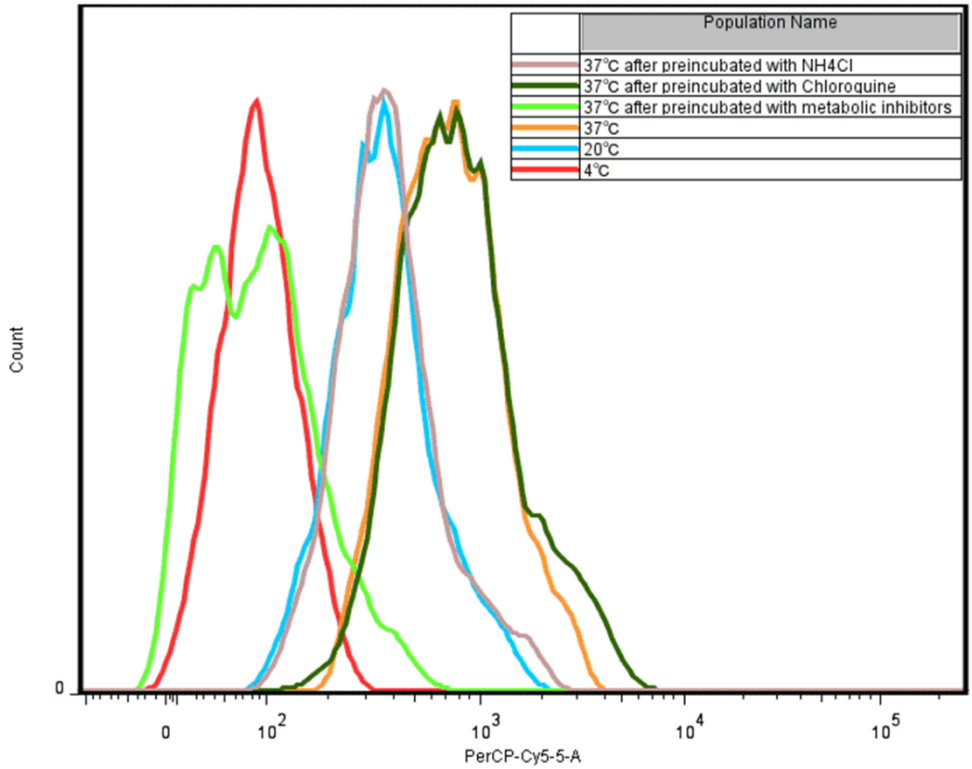


**Fig. S25** Flow cytometric histogram profile of cellular uptake of **MitoIr7** in HeLa cells. HeLa cells were incubated with 0.5 μM **MitoIr7** for 15 min at 37 °C (orange), 20°C (light blue), 4 °C (red), and 37 °C after the cells were preincubated with metabolic inhibitors 2-deoxy-D-glucose (50 mM) and oligomycin (5 μM) in PBS for 1 h at 37°C (light green), endocytic inhibitors $NH_4Cl$ (50 mM) (light purple) and chloroquine (50 μM) (dark green) in PBS for 1 h at 37°C, respectively.

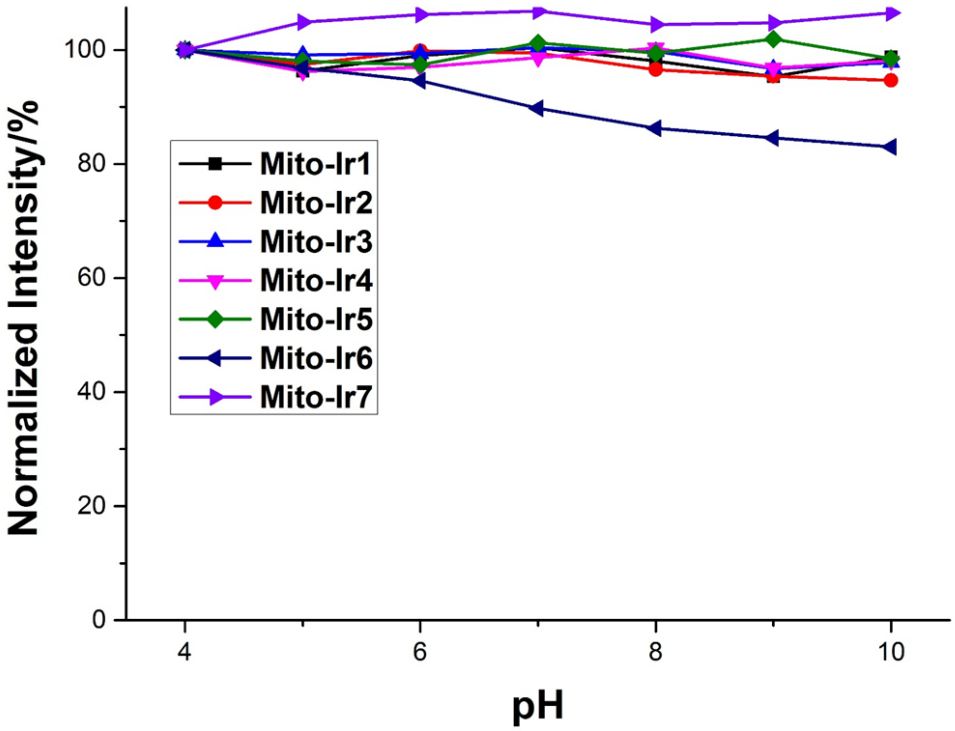


**Fig. S26** Emission intensity of 5 μM **MitoIr1-MitoIr7** at 595 nm under different pH in a Britton-Robinson buffer.

**Table S1** Photophysical data of **MitoIr1-MitoIr7**.

| Complexes | $\lambda_{abs}$/nm | $\lambda_{em}$//nm | τ/ns | Φ |
|---|---|---|---|---|
| **Ir1** | 253, 286, 383 | 598 | 94.5 | 0.108 |
| **Ir2** | 253, 287, 384 | 599 | 90.7 | 0.221 |
| **Ir3** | 253, 288, 383 | 596 | 85.9 | 0.219 |
| **Ir4** | 254, 288, 383 | 597 | 85.2 | 0.098 |
| **Ir5** | 253, 383 | 593 | 89.3 | 0.216 |
| **Ir6** | 254, 382 | 594 | 93.0 | 0.057 |
| **Ir7** | 288, 254, 383 | 590 | 91.2 | 0.365 |