

Supporting Information

Fluorinated cyclometalated iridium(III) complexes as mitochondria-targeted theranostic anticancer agents

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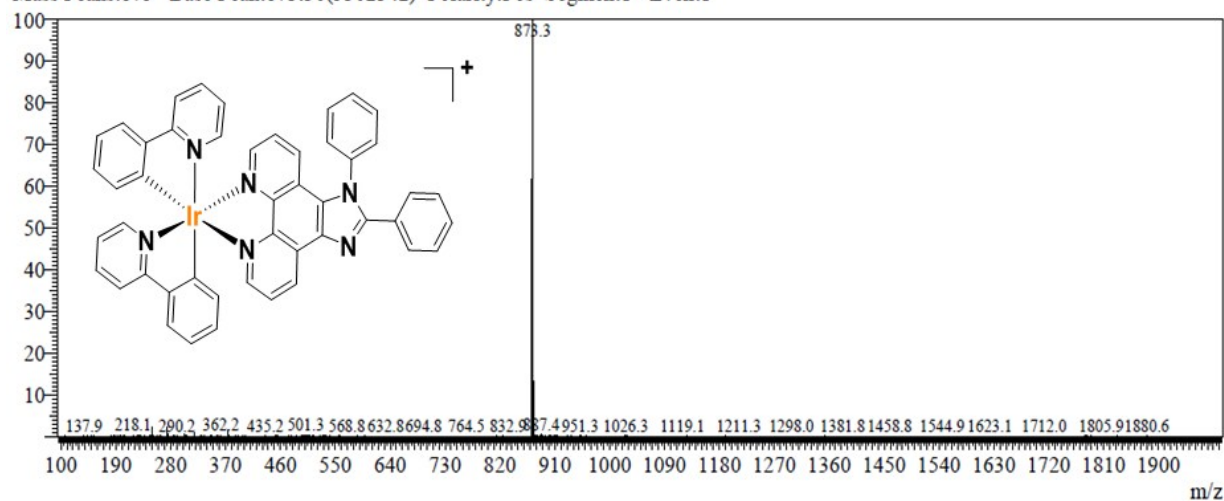


Fig. S1 ESI-MS spectra of Ir1 in CH₃OH solutions.

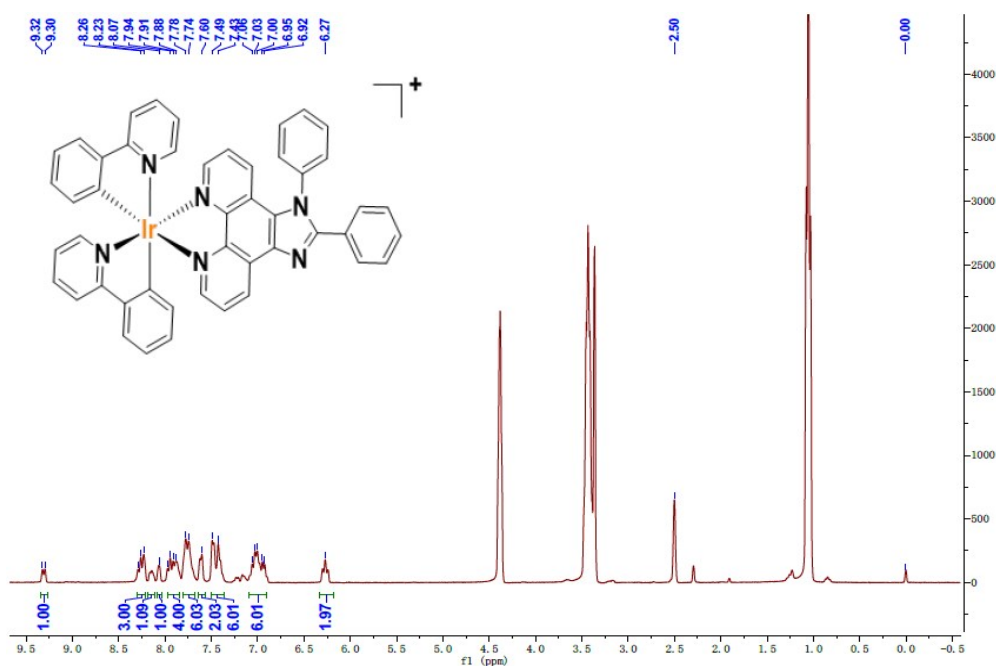


Fig. S2 ¹H NMR spectra of Ir1 in DMSO-d₆, 300 MHz.

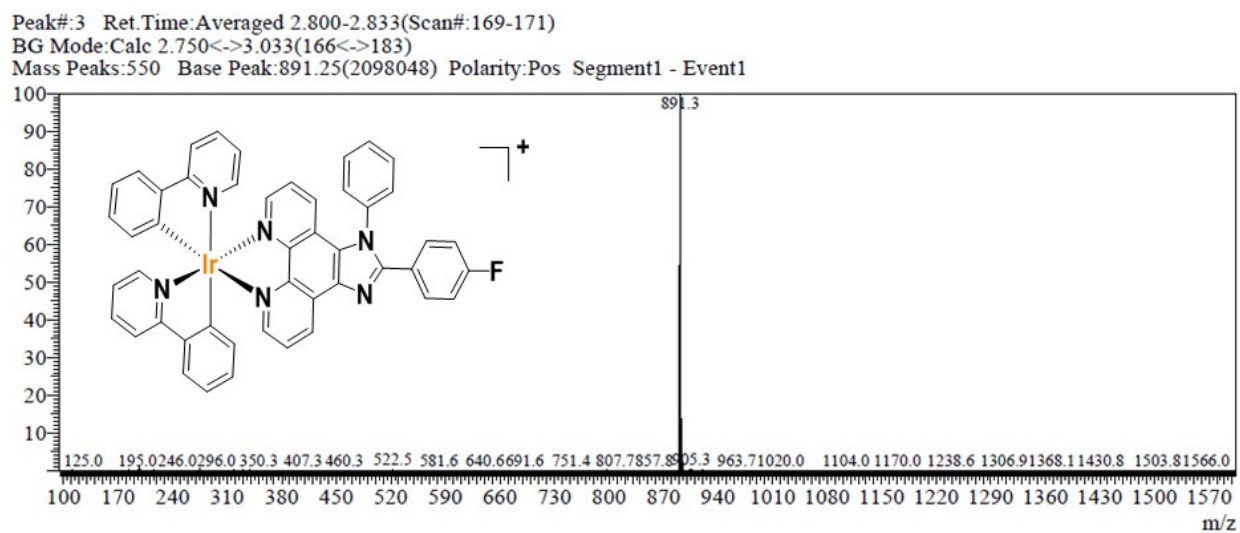


Fig. S3 ESI-MS spectra of Ir2 in CH₃OH solutions.

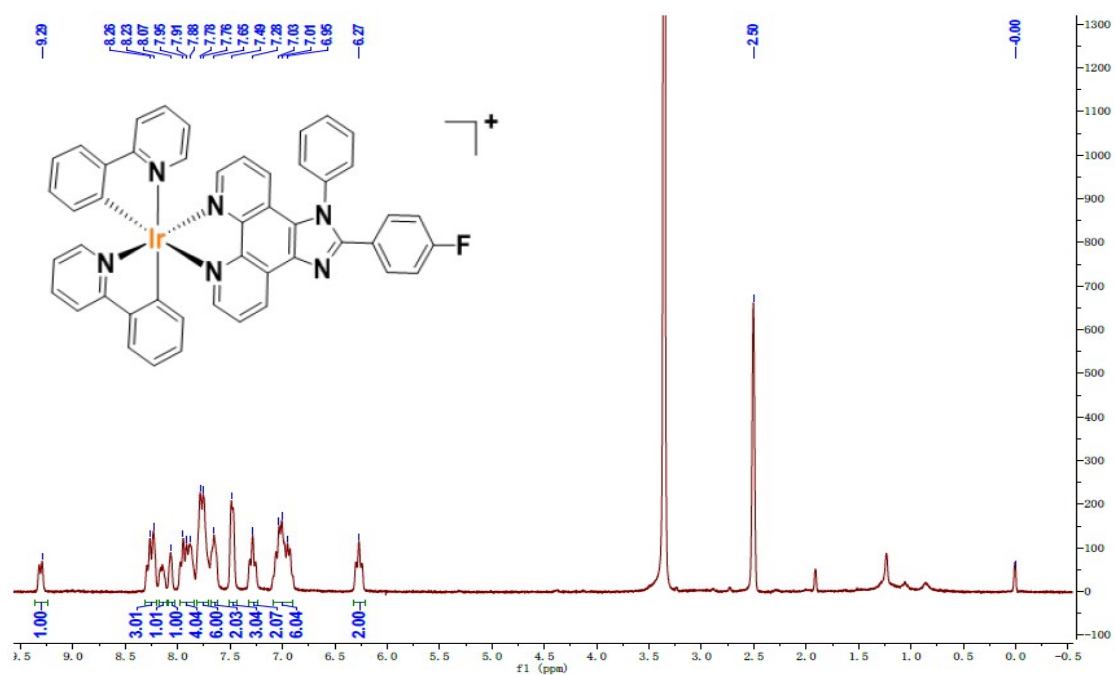


Fig. S4 ¹H NMR spectra of Ir2 in DMSO-d₆, 300 MHz.

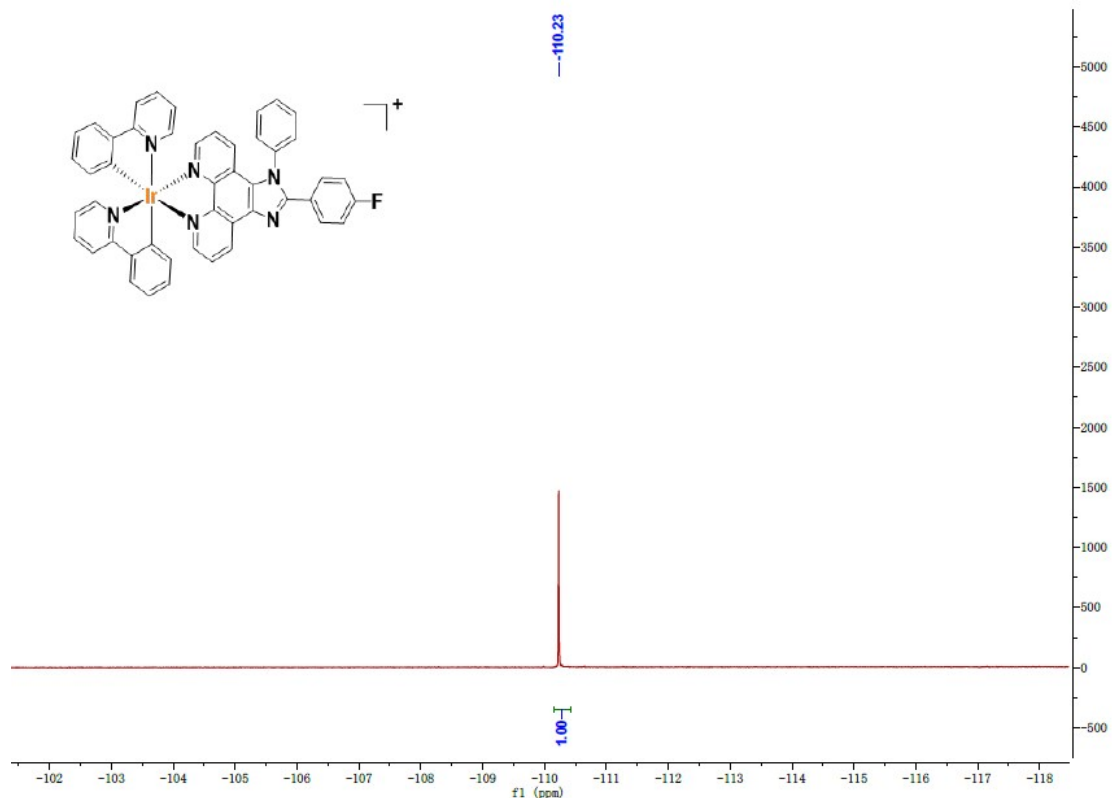


Fig. S5 ^{19}F NMR spectra of **Ir2** in DMSO-d_6 , 377 MHz.

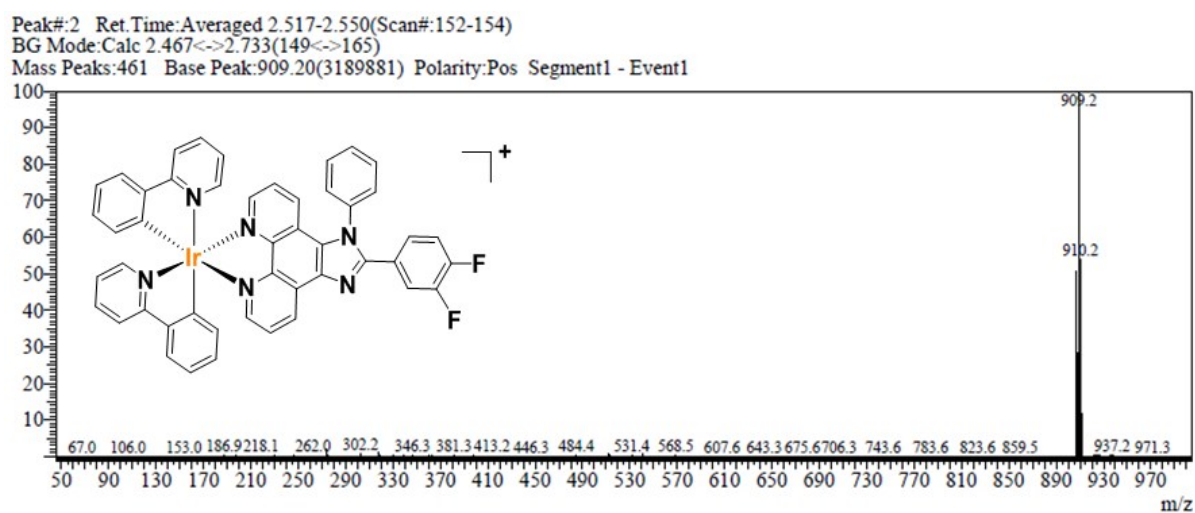


Fig. S6 ESI-MS spectra of **Ir3** in CH_3OH solutions.

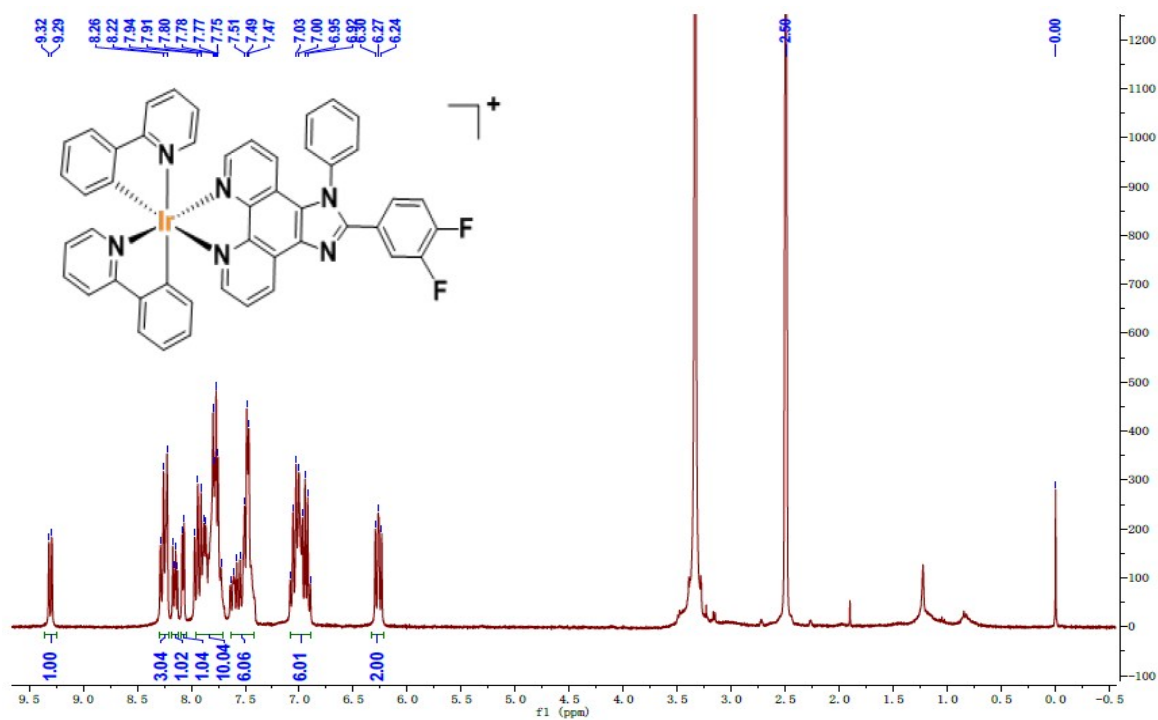


Fig. S7 ¹H NMR spectra of **Ir3** in DMSO-d₆, 300 MHz.

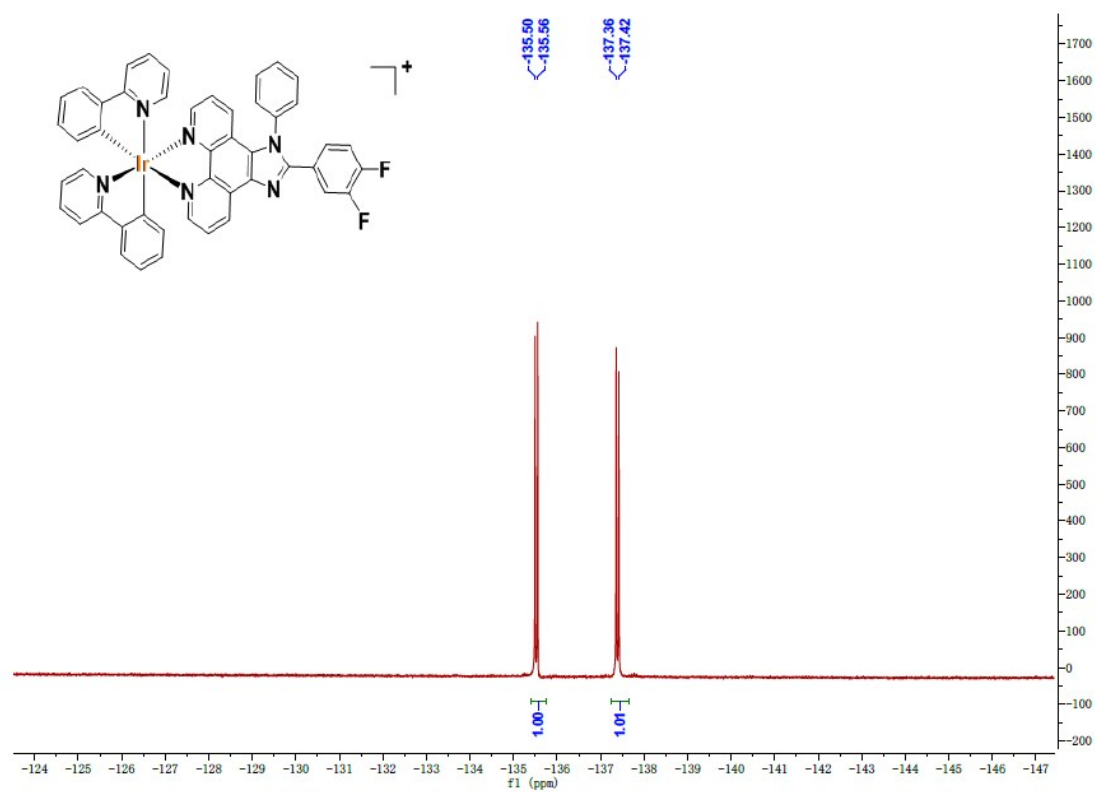


Fig. S8 ¹⁹F NMR spectra of **Ir3** in DMSO-d₆, 377 MHz.

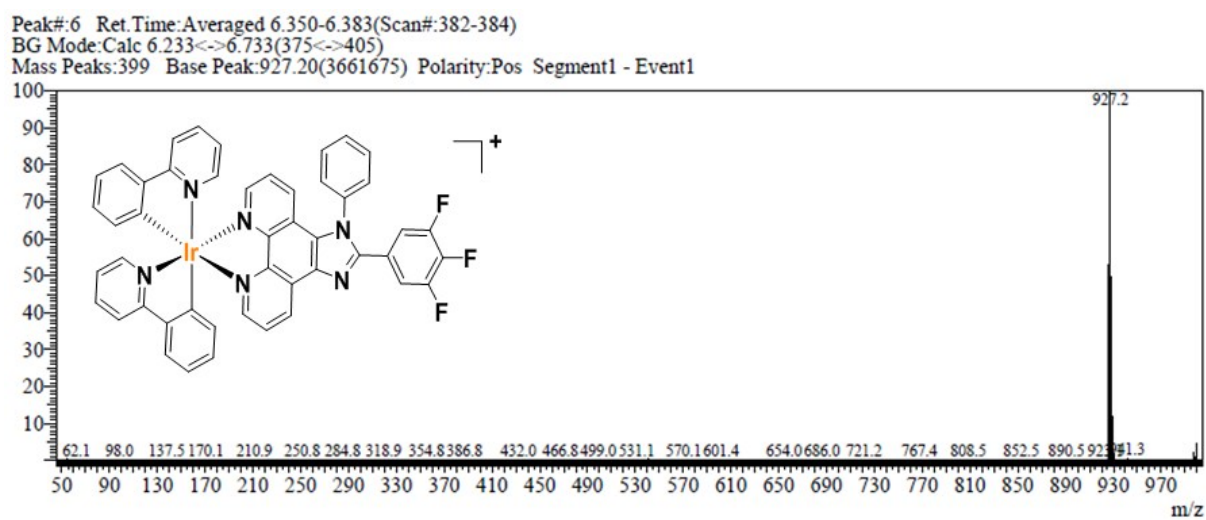


Fig. S9 ESI-MS spectra of Ir4 in CH₃OH solutions.

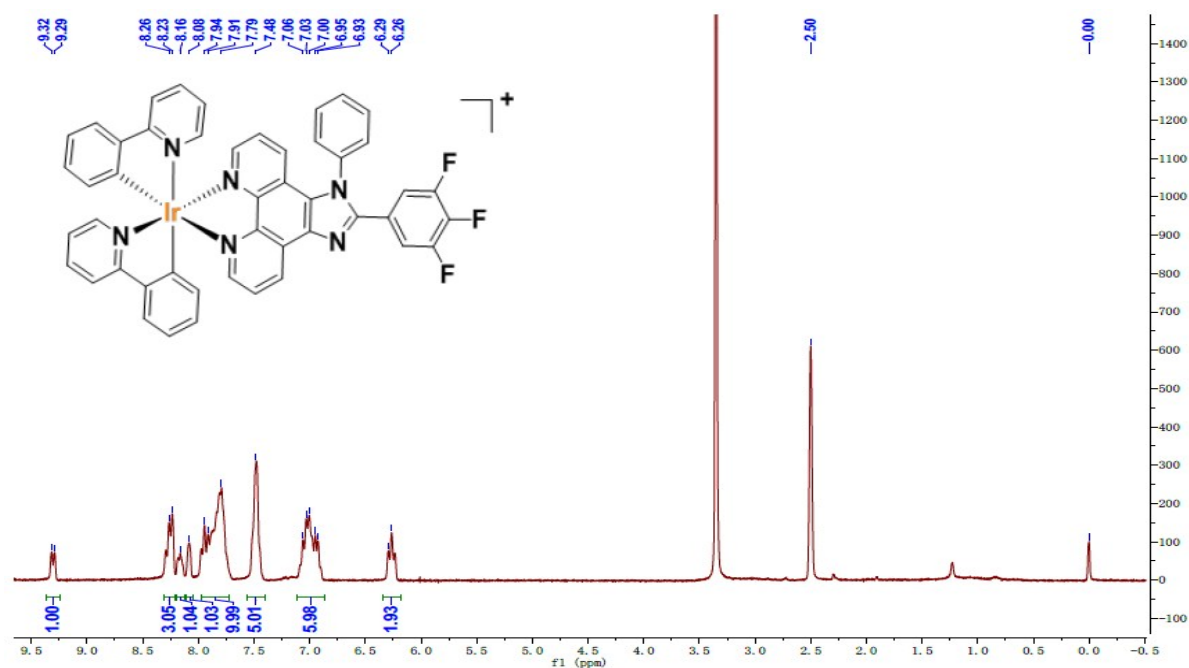


Fig. S10 ¹H NMR spectra of Ir4 in DMSO-d₆, 300 MHz.

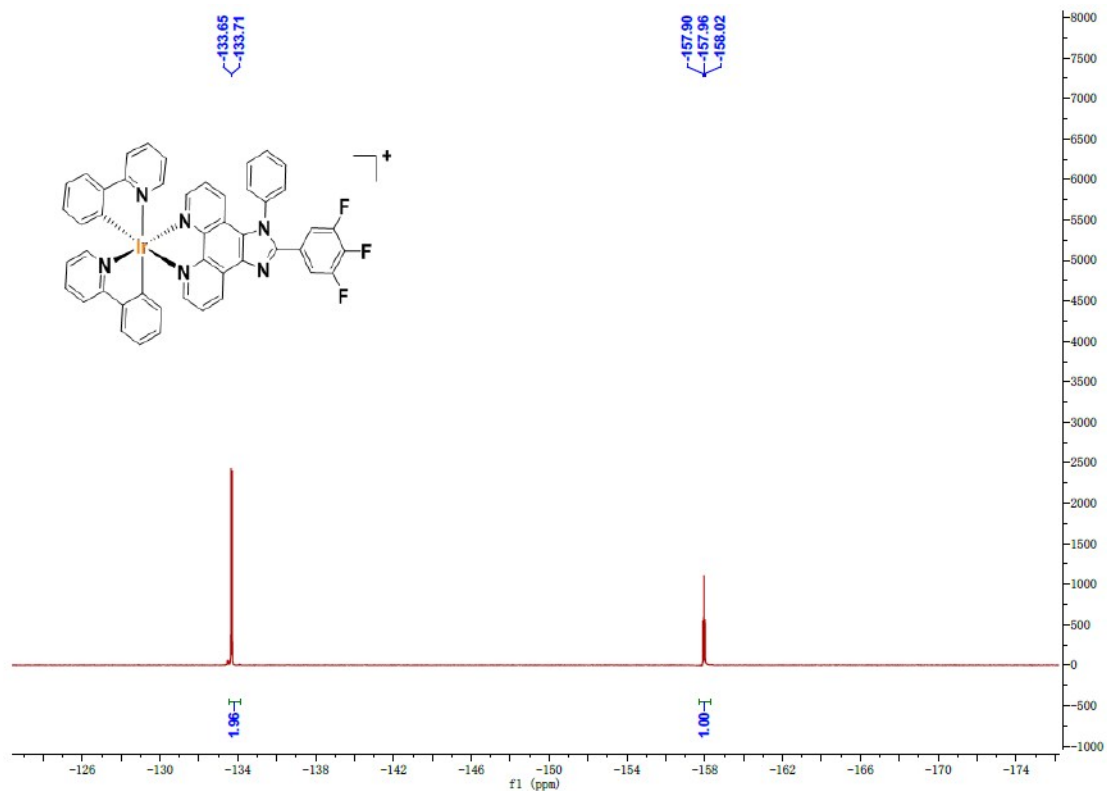


Fig. S11 ^{19}F NMR spectra of **Ir4** in DMSO-d_6 , 377 MHz.

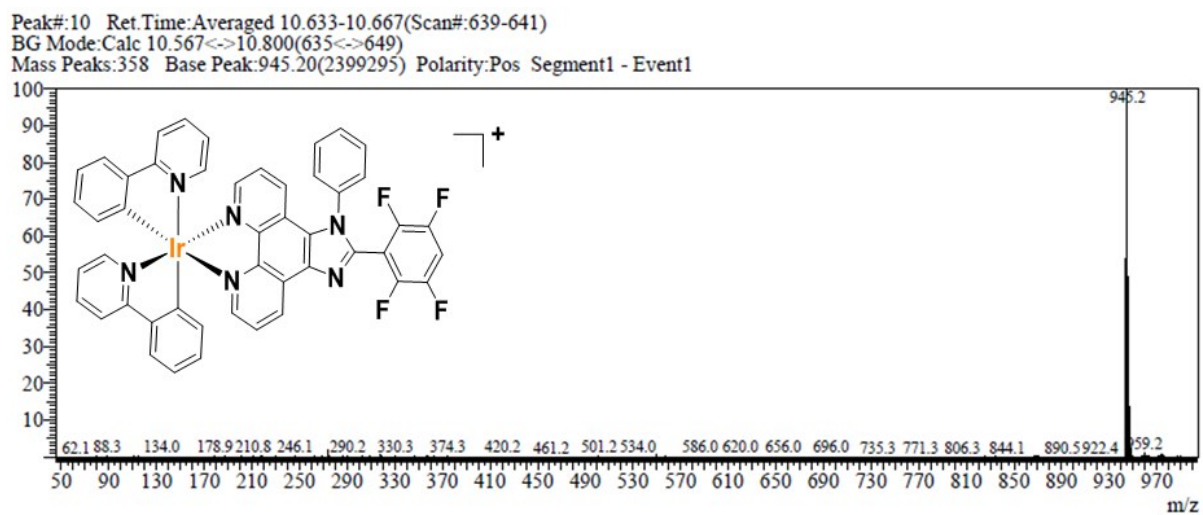


Fig. S12 ESI-MS spectra of **Ir5** in CH_3OH solutions.

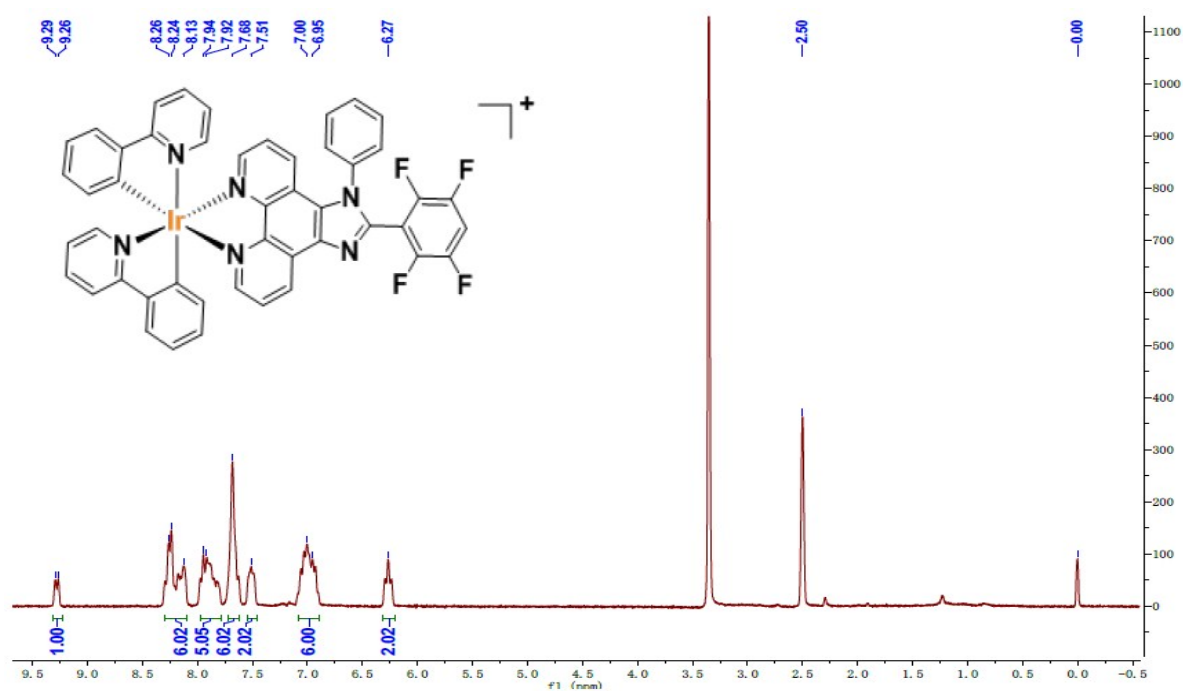


Fig. S13 ^1H NMR spectra of Ir5 in DMSO- d_6 , 300 MHz.

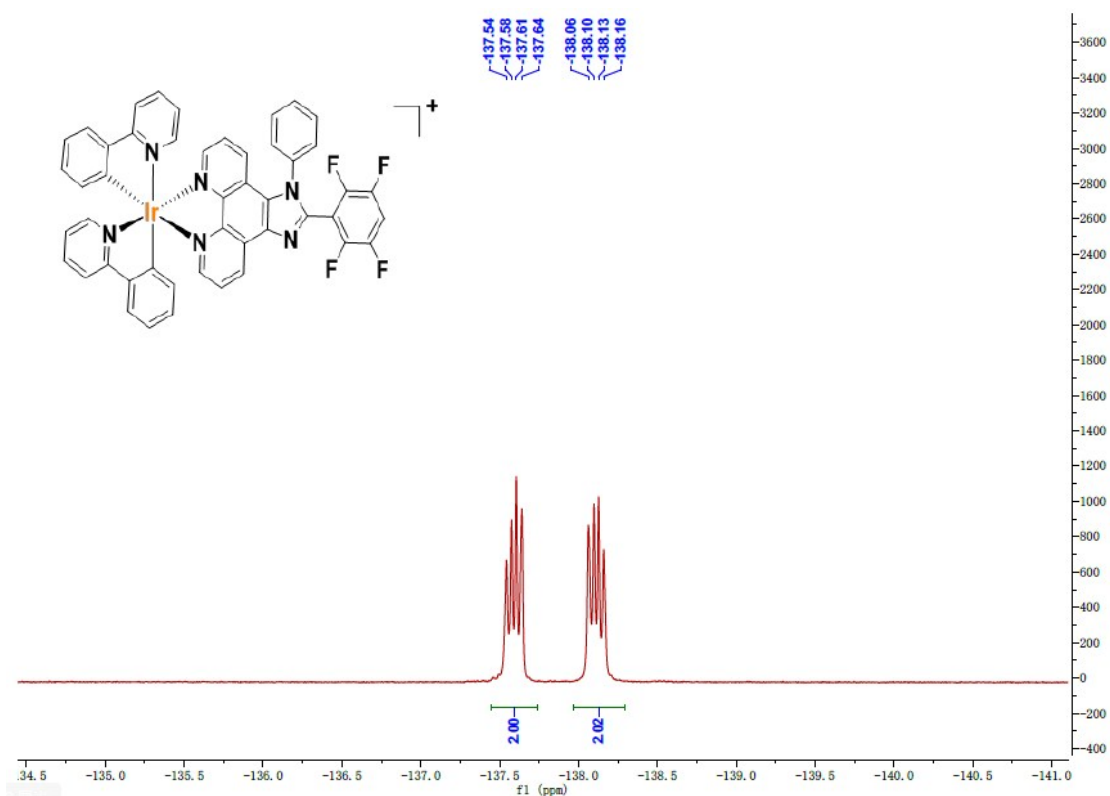


Fig. S14 ^{19}F NMR spectra of Ir5 in DMSO- d_6 , 377 MHz.

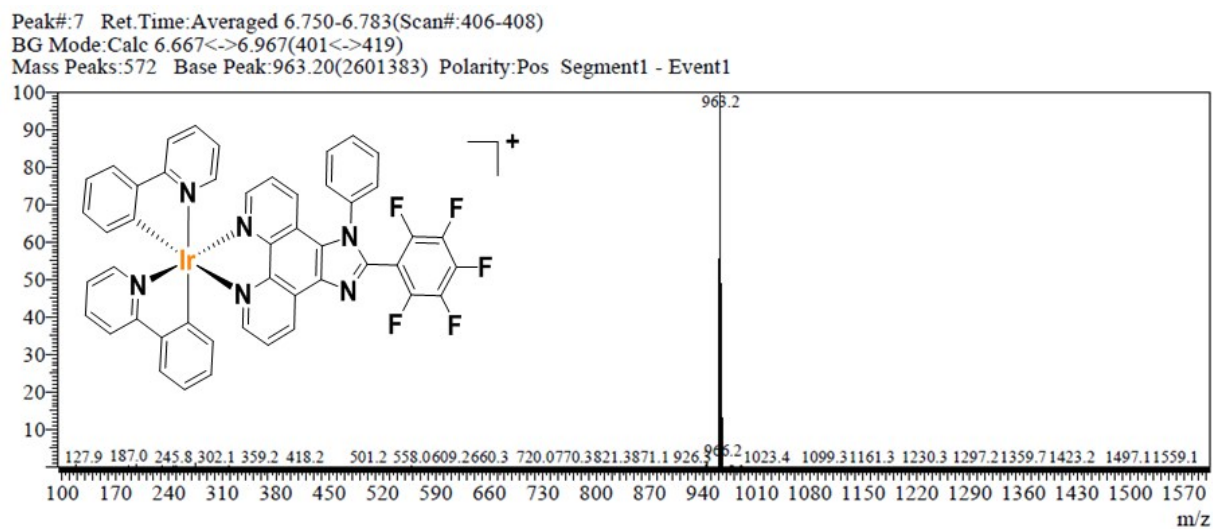


Fig. S15 ESI-MS spectra of Ir6 in CH₃OH solutions.

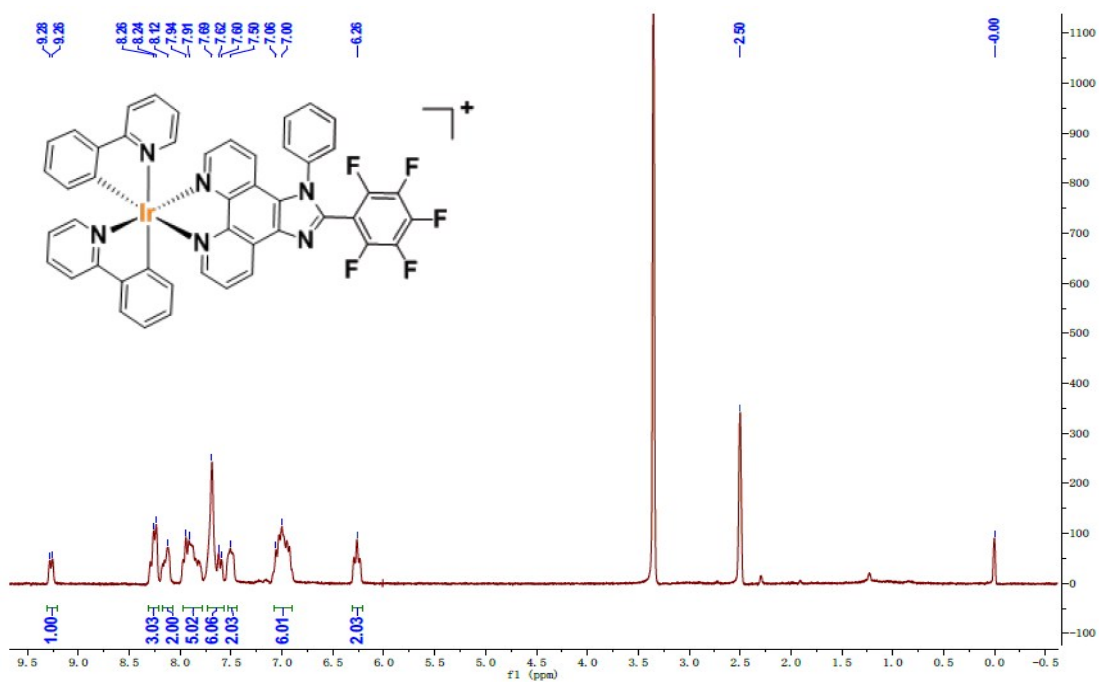


Fig. S16 ¹H NMR spectra of Ir6 in DMSO-d₆, 300 MHz.

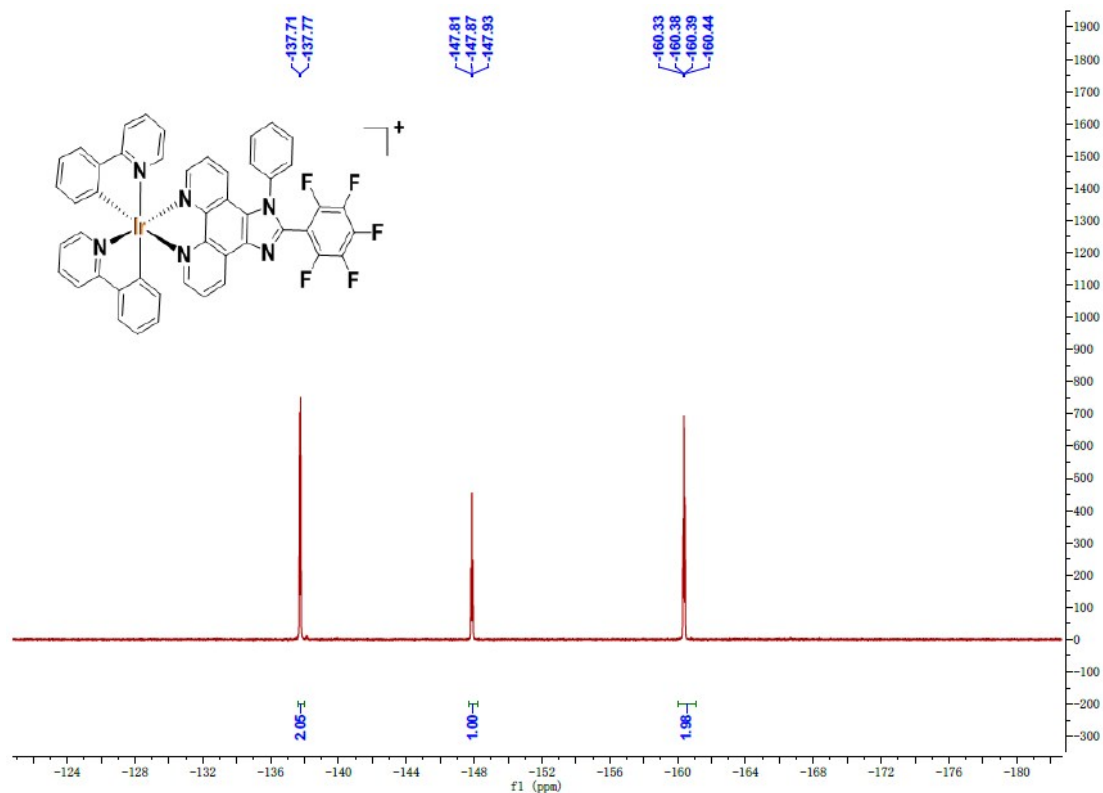


Fig. S17 ^{19}F NMR spectra of **Ir6** in DMSO-d_6 , 377 MHz.

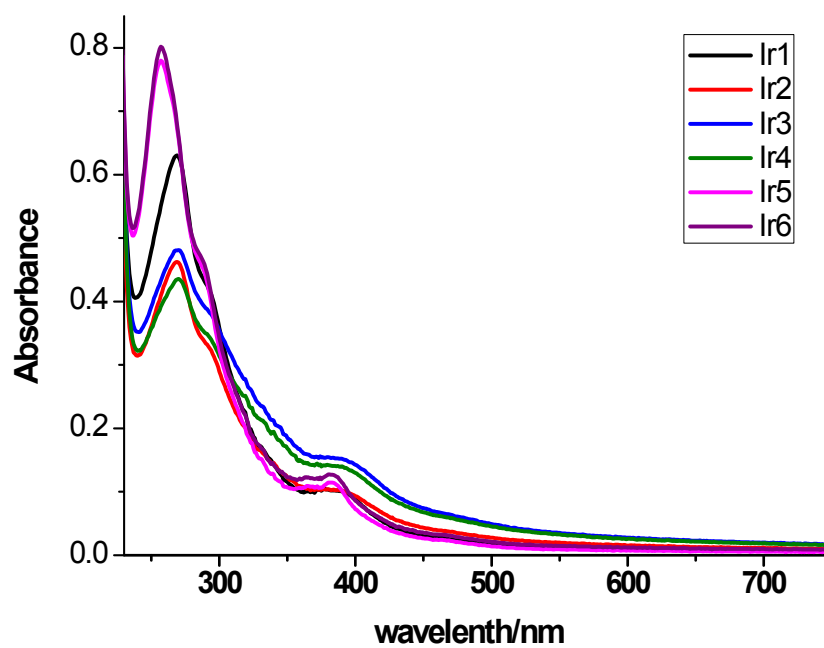


Fig. S18 Absorption spectra of **Ir1-Ir6** ($10\ \mu\text{M}$) in CH_2Cl_2 solution at 298K

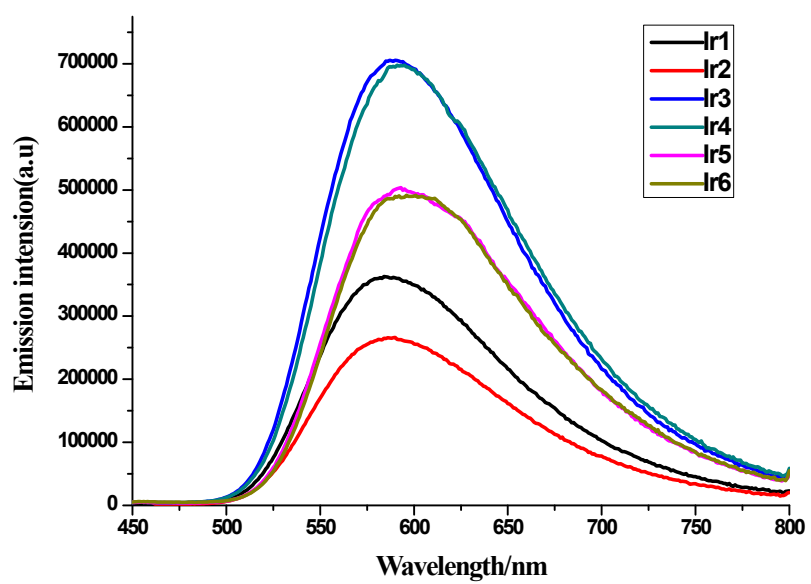


Fig. S19 Emission spectra of **Ir1-Ir6** (10 μ M) in CH₂Cl₂ solution at 298K with an excitation wavelength of 405 nm

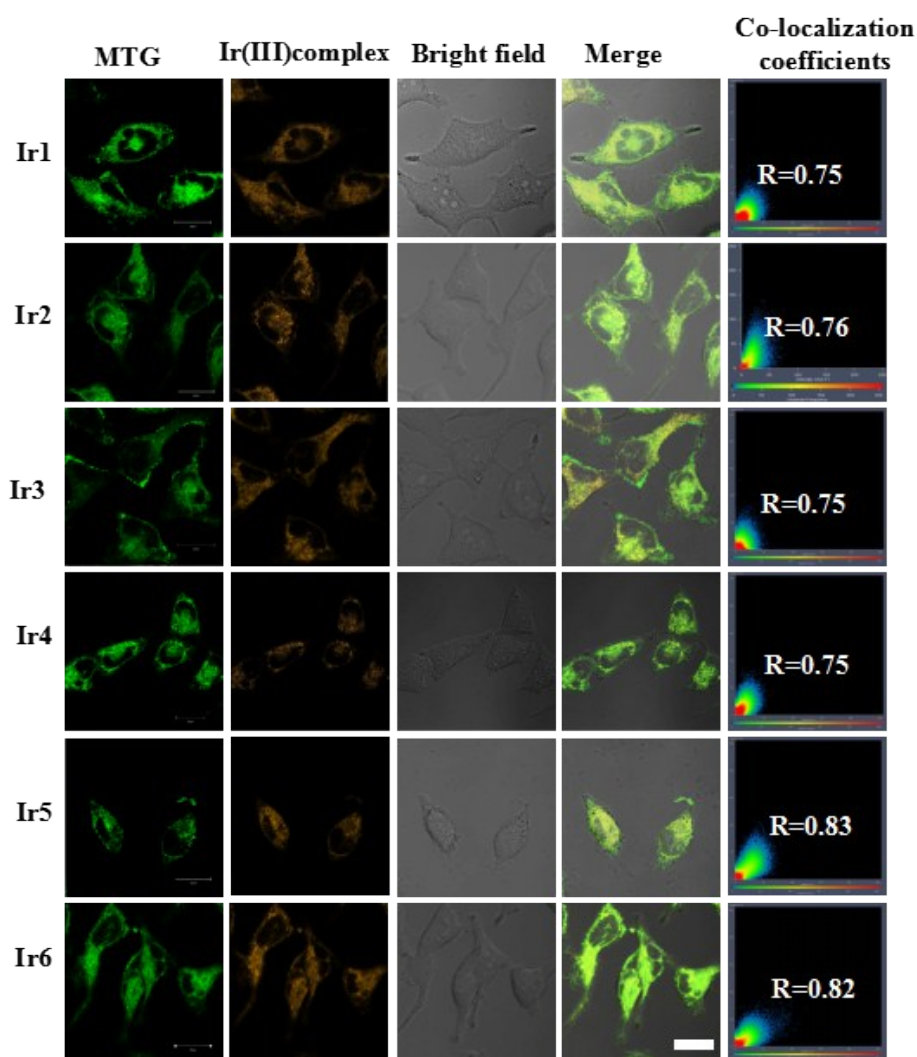


Fig. S20 Confocal fluorescence microscopy images of Hela cells colabeled with iridium(III) complexes ($0.5\mu\text{M}$, 15min) and MTG (150nM , 0.5h). Excitation wavelength: 405 nm (for all iridium(III) complexes), 488 nm (for MTG); emission filter: $580\pm 20\text{nm}$ (for all iridium(III) complexes) and $520\pm 20\text{nm}$ (for MTG). Cells shown were representative images from replicate experiments Cells shown were representative images from replicate experiments ($n=3$). Scale bar: $20\mu\text{m}$.

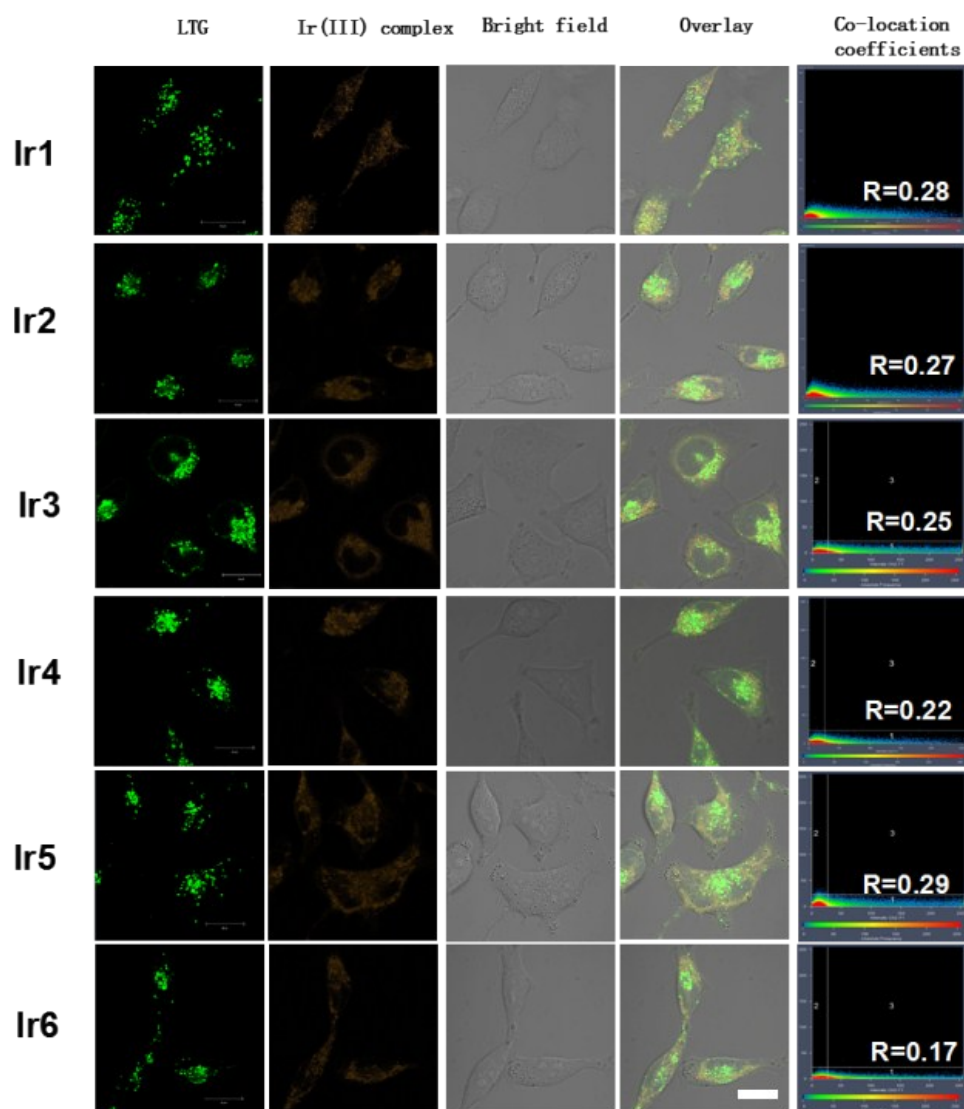


Fig. S21 Confocal fluorescence microscopy images of Hela cells colabeled with iridium(III) complexes(0.5 μ M, 15 min) and LTG (150 nM, 0.5 h). iridium(III) complexes Excitation wavelength: 405 nm (for all iridium(III) complexes), 488 nm(for LTG); emission filter: 580 $\pm$ 20 nm(for all iridium(III) complexes) and 510 $\pm$ 20 nm (for LTG). Cells shown were representative images from replicate experiments (n=3). Scale bar: 20 μ m.

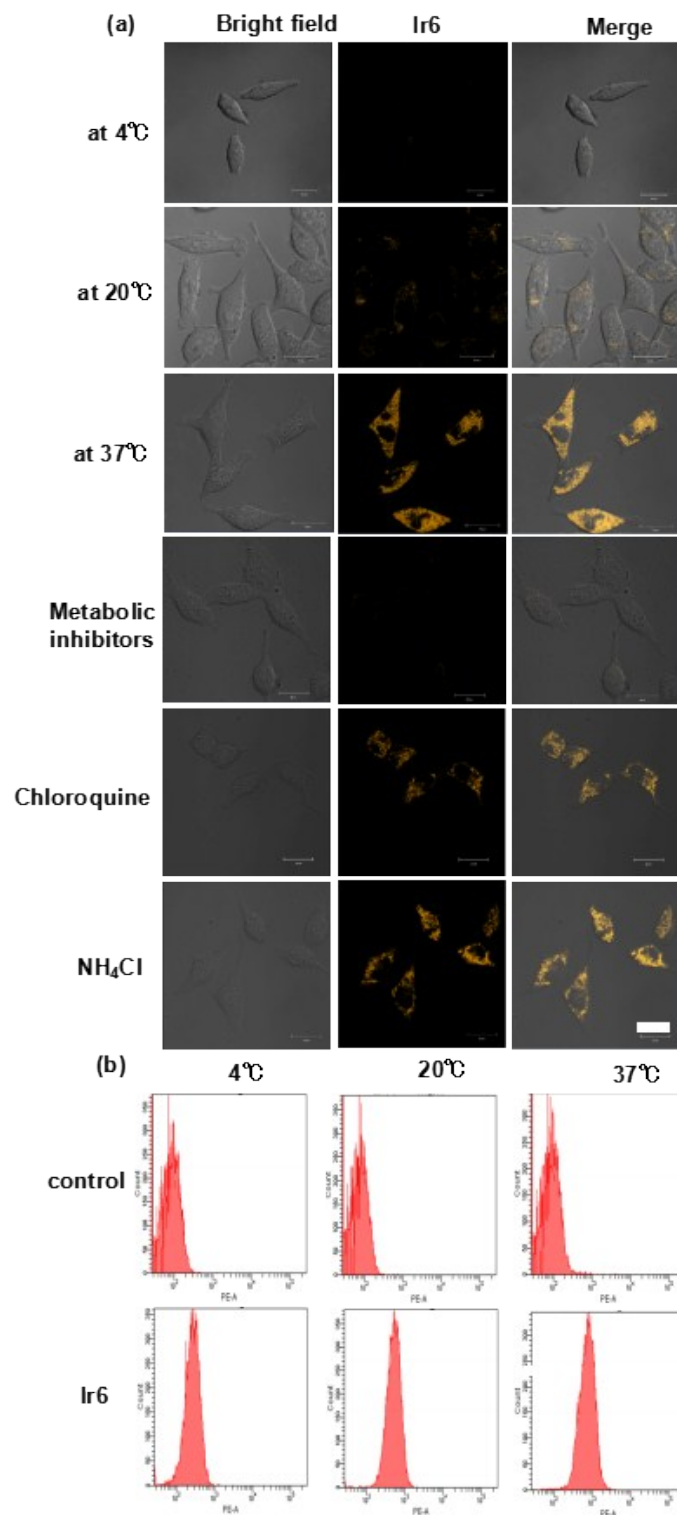


Fig. S22 (a) Confocal luminescence image and bright-field images of living HeLa cells incubated with 0.5 μM **Ir6** in DMSO–PBS (pH 7.4, 1:99,v/v) under different conditions. (b) Flow cytometry Scattergram showing the effect of the temperature on the uptake of **Ir6** (0.5 μM) in HeLa cells for 15 min.

Table S1 Photophysical data of **Ir1-Ir6** (in CH₂Cl₂).

Complexes	$\lambda_{\text{abs}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	τ/ns	Φ
Ir1	270, 383	587	191	0.028
Ir2	270, 387	588	179	0.039
Ir3	270, 381	589	188	0.032
Ir4	271, 381	593	187	0.029
Ir5	257, 387	594	200	0.033
Ir6	257, 388	600	191	0.025