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 CH$_3$OH solutions.

**Fig. S2** $^1$H NMR spectra of Ir1 in DMSO-d$_6$, 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$_3$OH solutions.
Fig. S7 $^1$H NMR spectra of Ir3 in DMSO-d$_6$, 300 MHz.

Fig. S8 $^{19}$F NMR spectra of Ir3 in DMSO-d$_6$, 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$_3$OH solutions.
Fig. S13 ¹H NMR spectra of Ir5 in DMSO-d₆, 300 MHz.

Fig. S14 ¹⁹F NMR spectra of Ir5 in DMSO-d₆, 377 MHz.
Fig. S15 ESI-MS spectra of Ir6 in CH$_3$OH solutions.

Fig. S16 $^1$H NMR spectra of Ir6 in DMSO-$d_6$, 300 MHz.
Fig. S17 $^{19}$F NMR spectra of Ir6 in DMSO-d$_6$, 377 MHz.

Fig. S18 Absorption spectra of Ir1-Ir6 (10 μM) in CH$_2$Cl$_2$ solution at 298K
**Fig. S19** Emission spectra of **Ir1-Ir6** (10 μM) 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 (0.5μM, 15min) and MTG (150nM, 0.5h). Excitation wavelength: 405 nm (for all iridium(III) complexes), 488 nm (for MTG); emission filter: 580±20nm (for all iridium(III) complexes) and 520±20nm (for MTG). Cells shown were representative images from replicate experiments (n=3). Scale bar: 20 μm.
Fig. S21 Confocal fluorescence microscopy images of Hela cells colabeled with iridium(III) complexes (0.5 μM, 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±20 nm (for all iridium(III) complexes) and 510±20 nm (for LTG). Cells shown were representative images from replicate experiments (n=3). Scale bar: 20 μm.
Fig. S22 (a) Confocal luminescence image and bright-field images of living HeLa cells incubated with 0.5 $\mu$M 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 $\mu$M) in HeLa cells for 15 min.
### Table S1 Photophysical data of **Ir1-Ir6** (in CH$_2$Cl$_2$).

<table>
<thead>
<tr>
<th>Complexes</th>
<th>$\lambda_{\text{abs}}$/nm</th>
<th>$\lambda_{\text{em}}$/nm</th>
<th>$\tau$/ns</th>
<th>$\Phi$</th>
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</thead>
<tbody>
<tr>
<td><strong>Ir1</strong></td>
<td>270, 383</td>
<td>587</td>
<td>191</td>
<td>0.028</td>
</tr>
<tr>
<td><strong>Ir2</strong></td>
<td>270, 387</td>
<td>588</td>
<td>179</td>
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<td><strong>Ir3</strong></td>
<td>270, 381</td>
<td>589</td>
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</tr>
<tr>
<td><strong>Ir4</strong></td>
<td>271, 381</td>
<td>593</td>
<td>187</td>
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<tr>
<td><strong>Ir5</strong></td>
<td>257, 387</td>
<td>594</td>
<td>200</td>
<td>0.033</td>
</tr>
<tr>
<td><strong>Ir6</strong></td>
<td>257, 388</td>
<td>600</td>
<td>191</td>
<td>0.025</td>
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