

Supporting Information

**Endoplasmic reticulum targeted cyclometalated iridium(III)
complexes as efficient photodynamic therapy photosensitizers**

Bo Yuan,^a Jiangping Liu,^{*a} Ruilin Guan,^a Chengzhi Jin,^{*a} Liangnian Ji^a and Hui Chao^{*a,b}

^aMOE key laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry, Sun Yat-Sen University, Guangzhou 510275, P. R. China.

E-mail: ceshh@mail.sysu.edu.cn, ceslijiangping@foxmail.com, chengzhi.jin@yahoo.com

^bMOE Key Laboratory of Theoretical Organic Chemistry and Functional Molecule, School of Chemistry and Chemical Engineering, Hunan University of Science and Technology, Xiangtan, 400201, P. R. China

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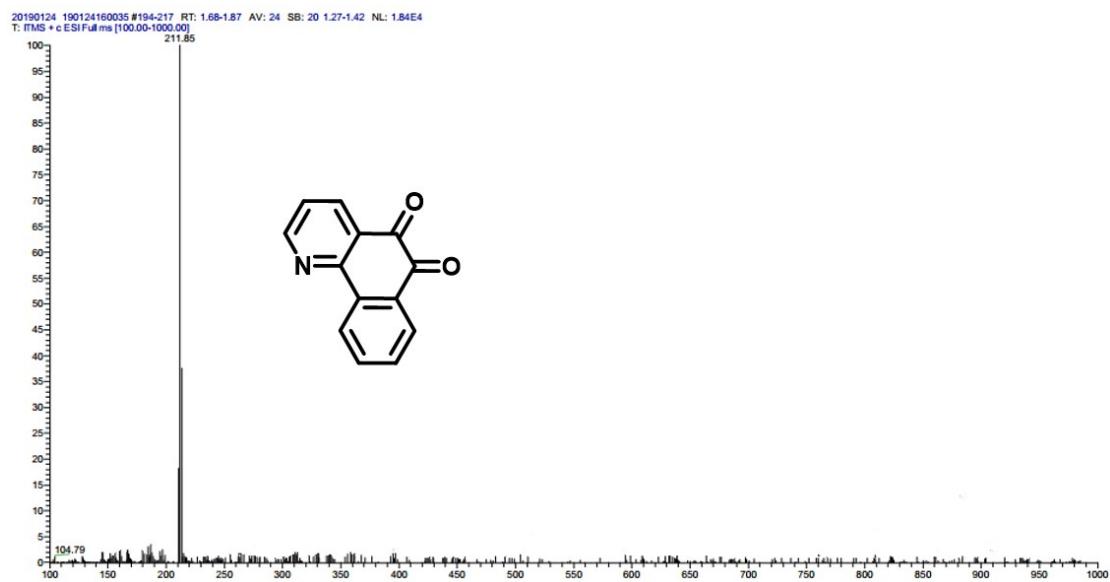


Fig. S1 ESI-MS of Benzo[h]quinoline-5,6-dione in CH_3OH

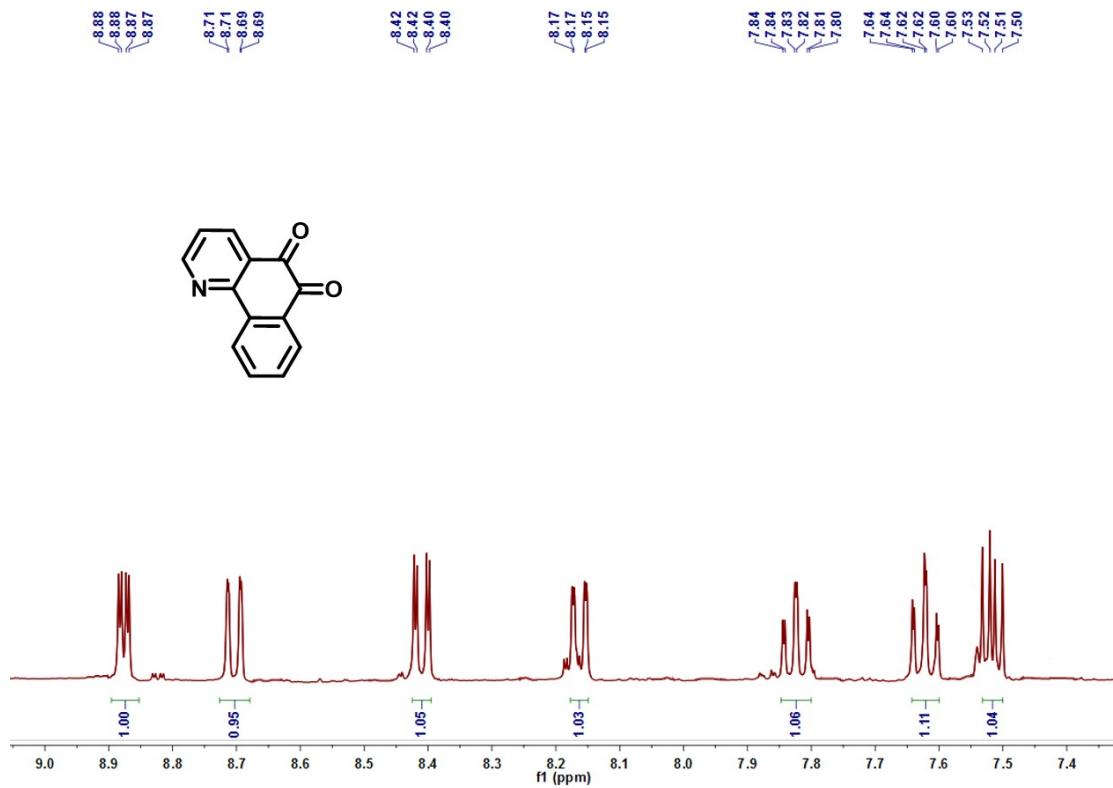


Fig. S2 ^1H NMR spectrum of Benzo[h]quinoline-5,6-dione in $\text{DMSO}-d_6$.

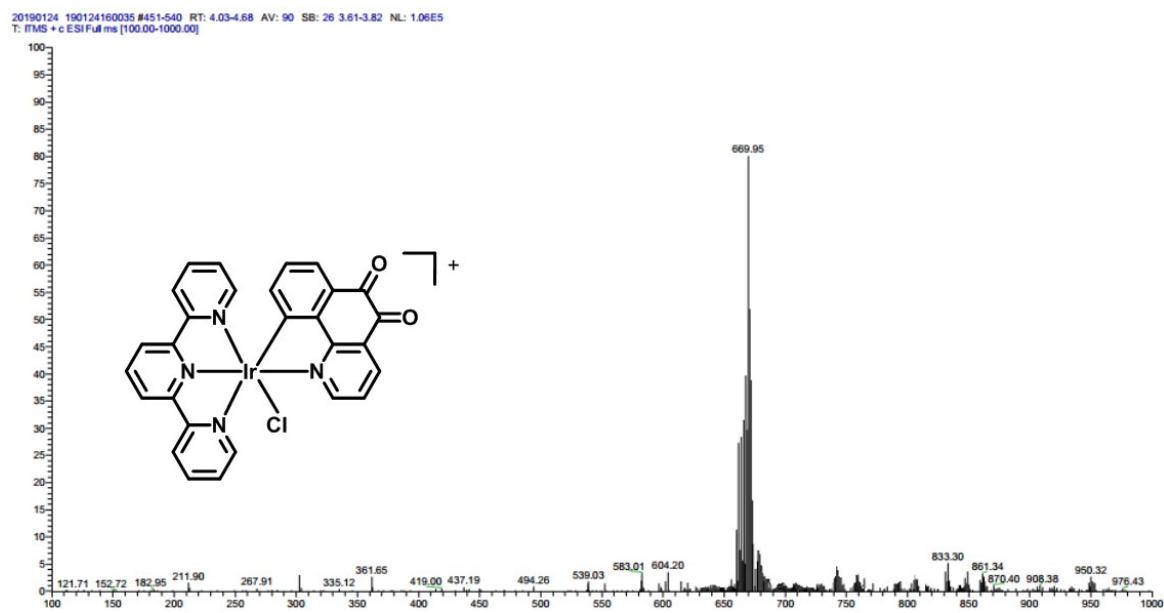


Fig. S3 ESI-MS of $[\text{Ir}(\text{tpy})(\text{bhqd})\text{Cl}] \text{PF}_6$ in CH_3OH

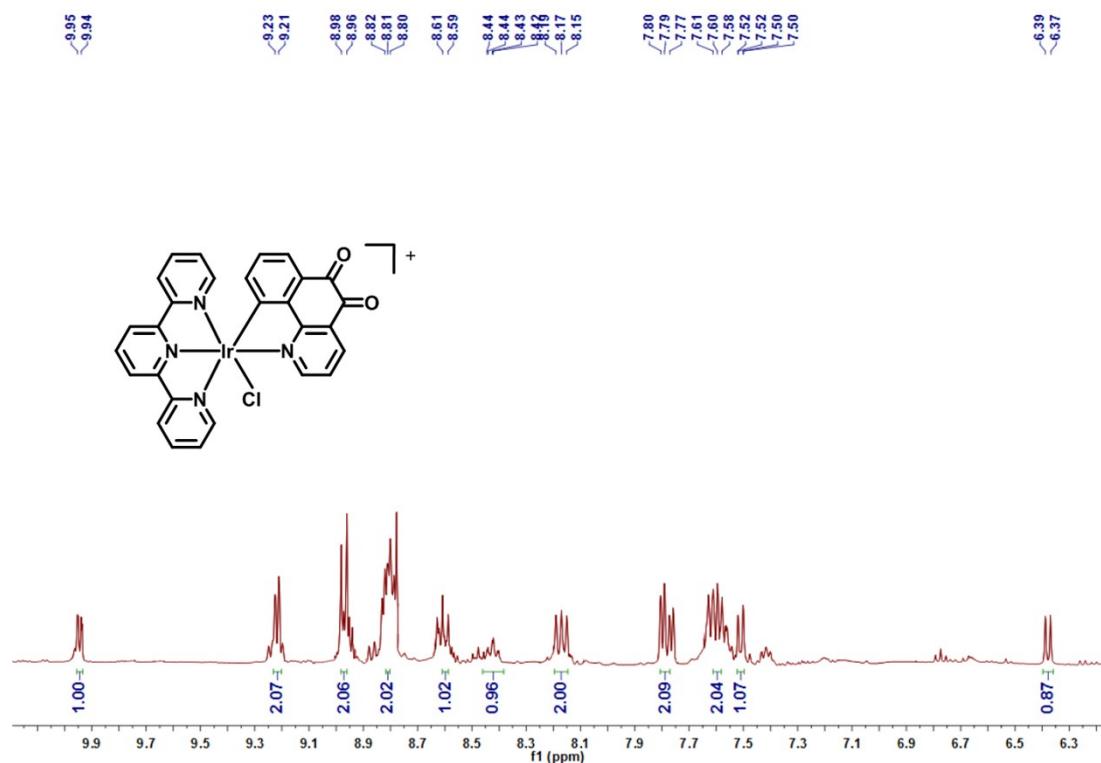


Fig. S4 ^1H NMR spectrum of $[\text{Ir}(\text{tpy})(\text{bhqd})\text{Cl}] \text{PF}_6$ in $\text{DMSO}-d_6$

Peak#:1 Ret.Time:Averaged 6.050-6.083(Scan#:364-366)
 BG Mode:Calc 6.000<->6.183(361<->372)
 Mass Peaks:833 Base Peak:691.00(335738) Polarity:Pos Segment1 - Event1

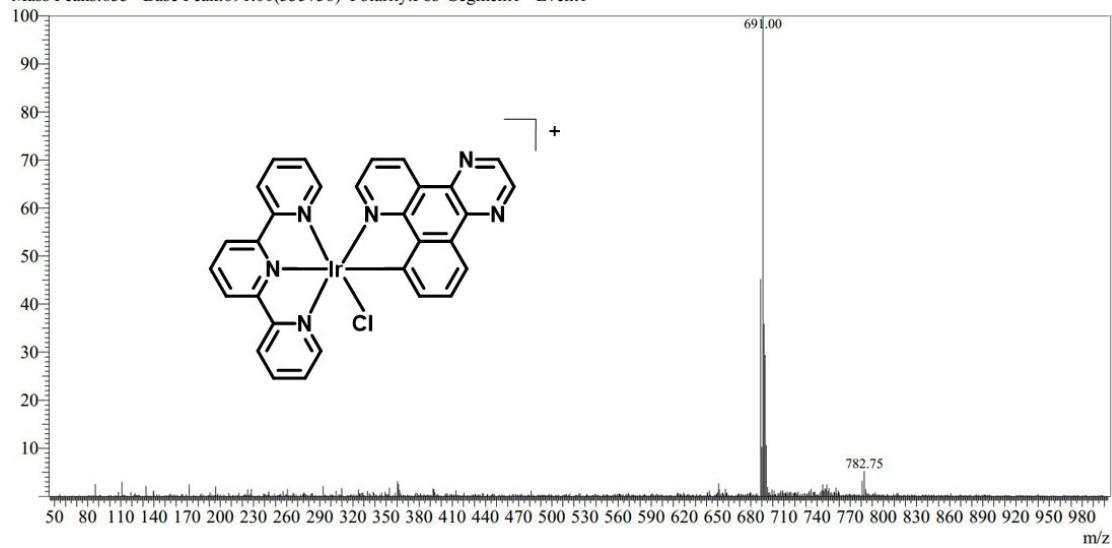


Fig. S5 ESI-MS of Ir1 in CH₃OH

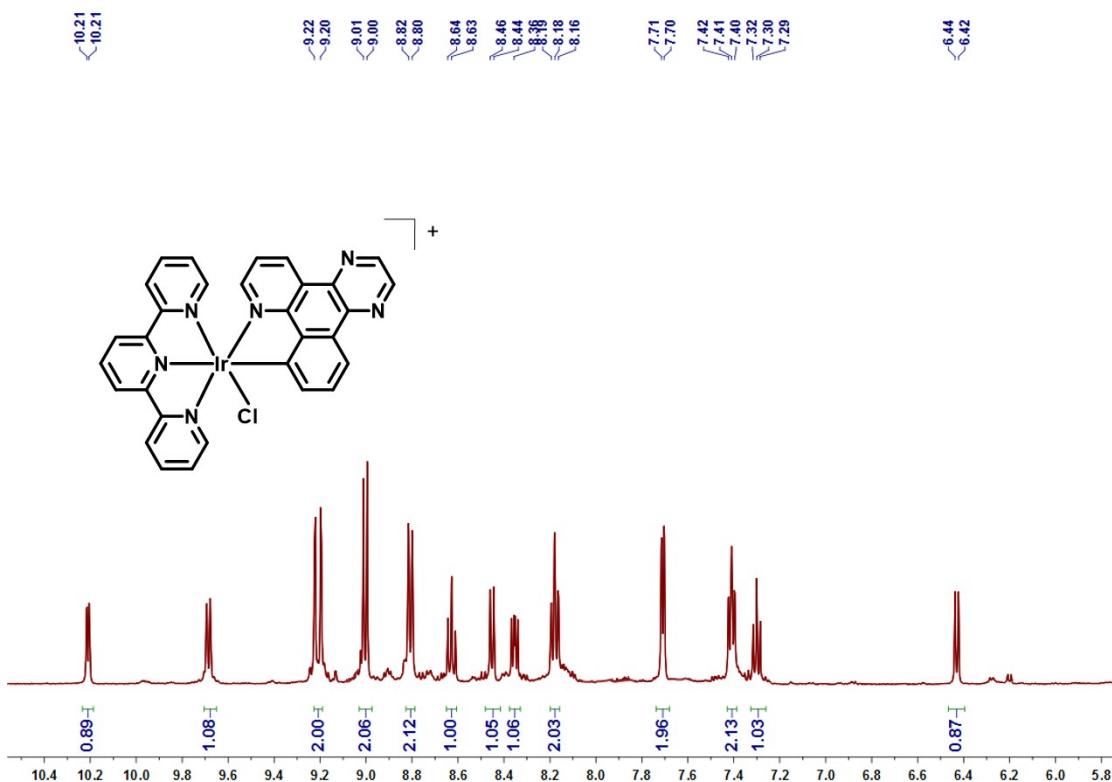


Fig. S6 ¹H NMR spectrum of Ir1 in DMSO-*d*₆

Peak#:1 Ret.Time:Averaged 2.867-2.900(Scan#:173-175)
 BG Mode:Calc 2.800<->3.033(169<->183)
 Mass Peaks:272 Base Peak:741.00(294293) Polarity:Pos Segment1 - Event1

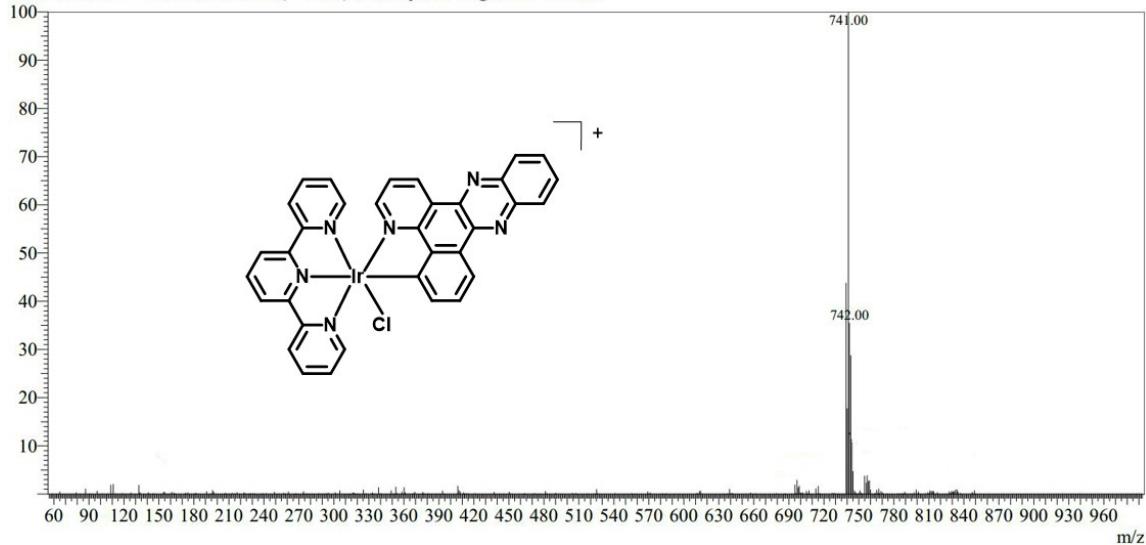


Fig. S7 ESI-MS of Ir2 in CH_3OH

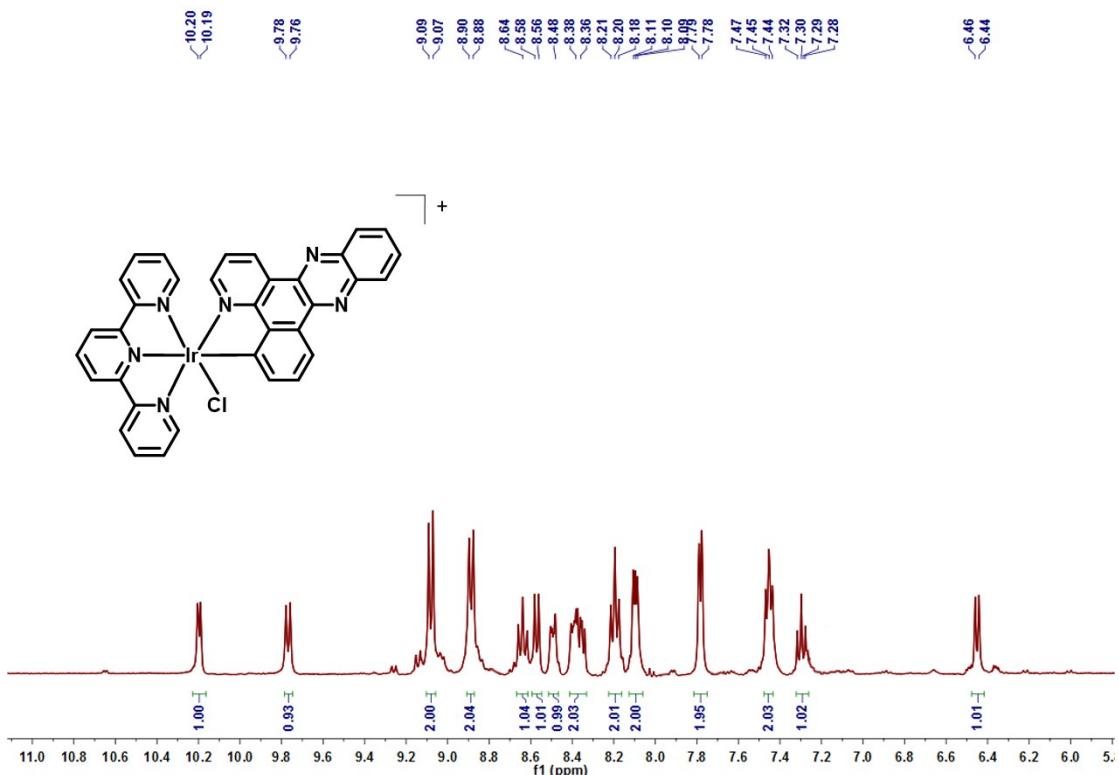


Fig. S8 ^1H NMR spectrum of Ir2 in $\text{DMSO}-d_6$

Peak#:1 Ret.Time:Averaged 4.333-4.367(Scan#:261-263)
 BG Mode:Calc 4.267<->4.517(257<->272)
 Mass Peaks:768 Base Peak:791.00(316288) Polarity:Pos Segment1 - Event1

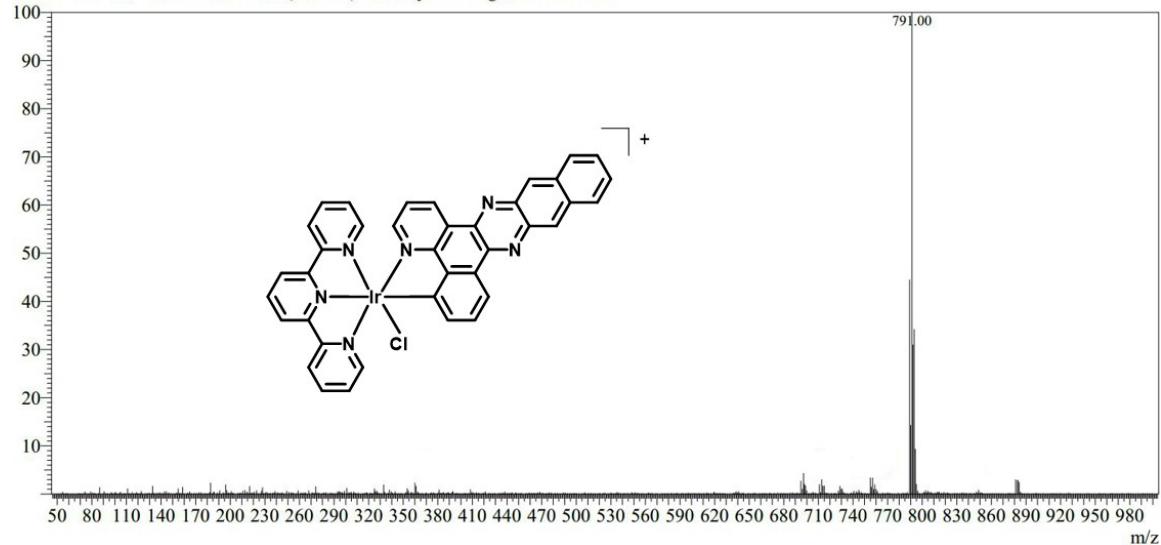


Fig. S9 ESI-MS of Ir3 in CH₃OH

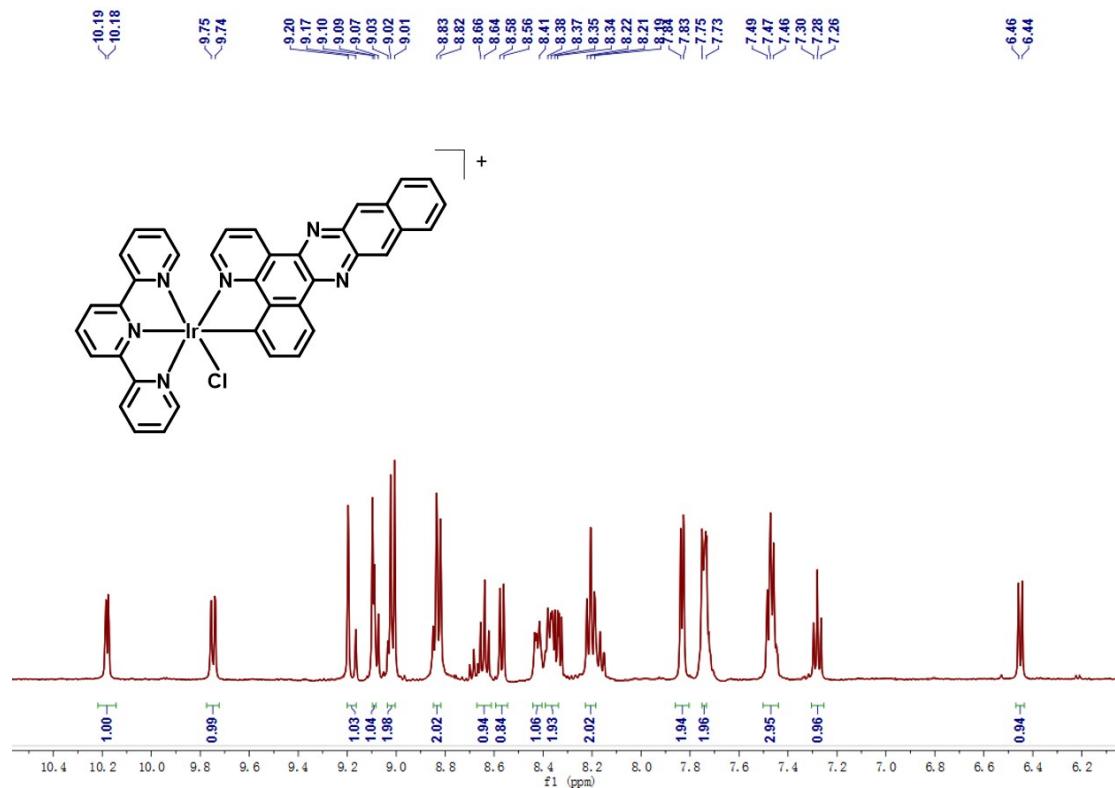


Fig. S10 ¹H NMR spectrum of Ir3 in DMSO-*d*₆

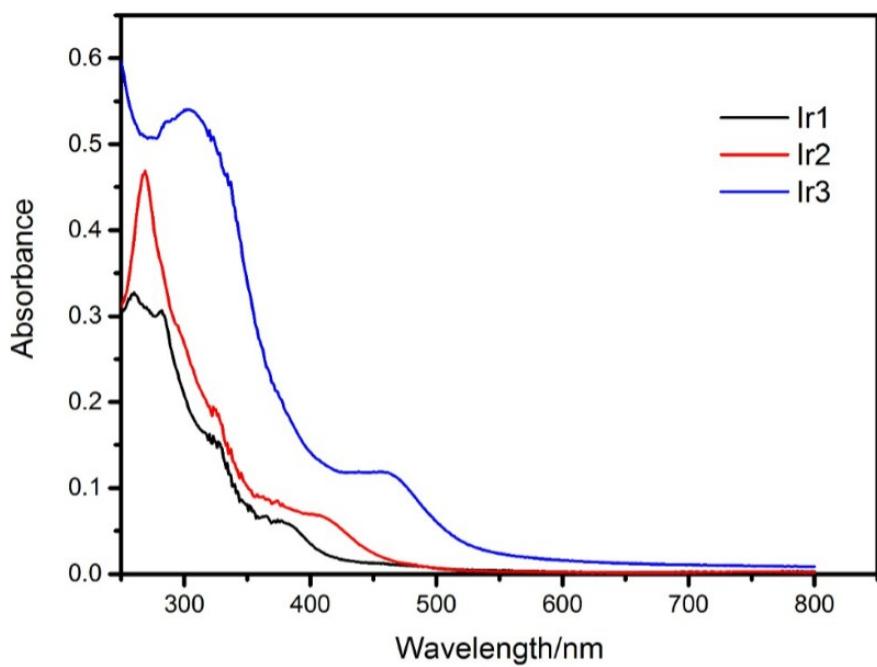


Fig. S11 The absorption spectra of **Ir1-Ir3** at 298 K in PBS.

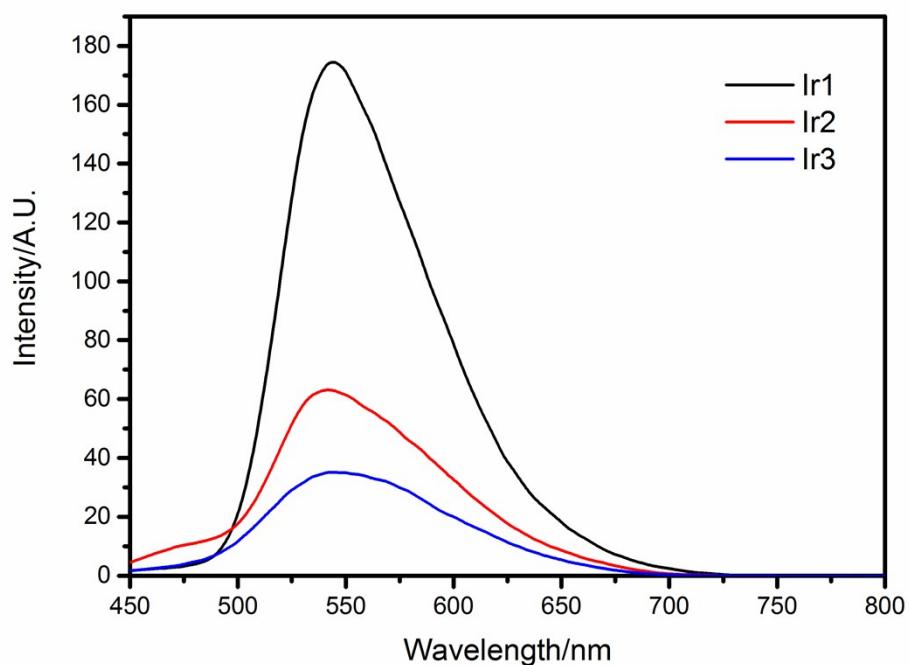


Fig. S12 The Emission spectra of **Ir1-Ir3** at 298 K in PBS.

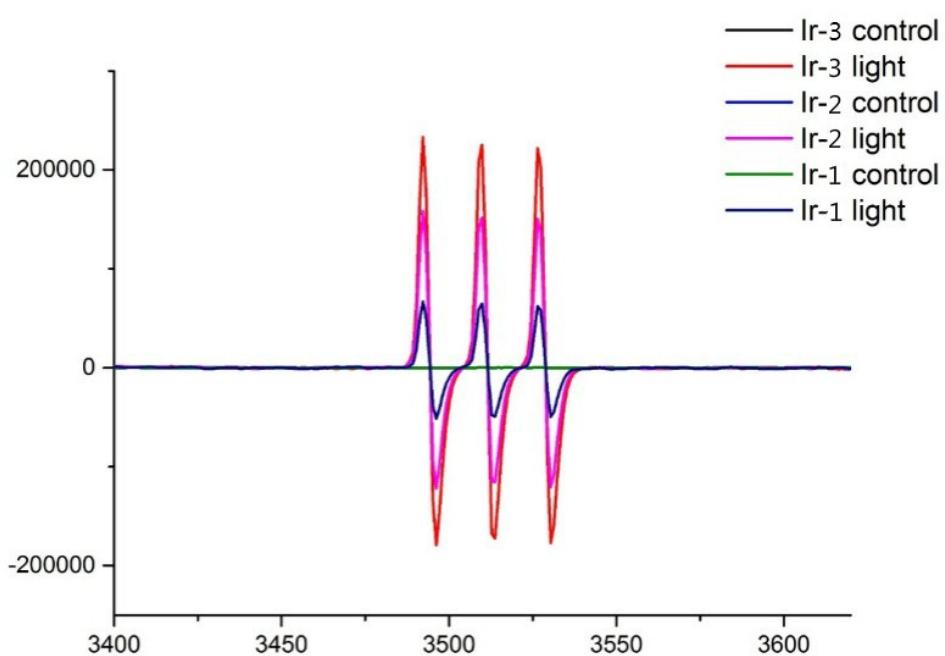


Fig. S13 The ESR spectra of **Ir1-3** with TEMP as singlet oxygen trap.

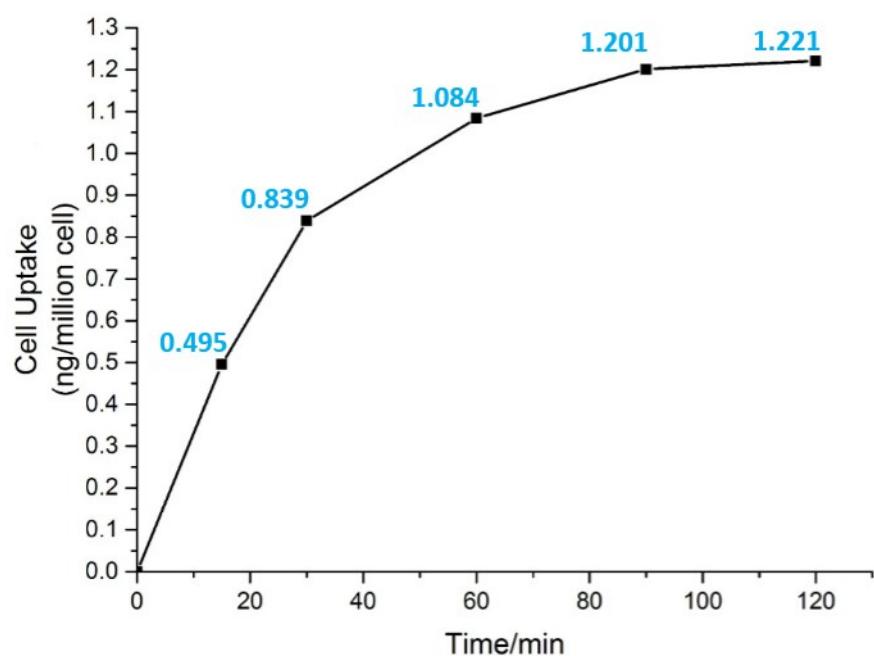


Fig. S14 Time-dependent cellular uptake of **Ir1-Ir3** by ICP-MS.

Table. S1 Photophysical properties of **Ir1-Ir3^a**

Complexes	$\lambda_{abs}/\text{nm}^b$	λ_{em}/nm^c	$\tau/\mu\text{s}^d$	Φ^e
Ir1	378	540	1.437	0.125
Ir2	421	538	1.031	0.056
Ir3	460	546	1.416	0.018

^a All data were obtained at 298 K in PBS.

^b Wavelength corresponding to the absorption maxima.

^c Wavelength corresponding to the emission maxima.

^d Lifetime in PBS.

^e Phosphorescence quantum yield.

Table. S2 $\log P_{o/w}$ of **Ir1-Ir3**

Ir1	Ir2	Ir3
-0.5334	-0.0466	0.1056