Supporting Information

N-Phenylcarbazole/Triphenylamine-modificated Half-Sandwich Iridium(III) Schiff Base Complexes and Anticancer Application

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1 Experimental Section

1.1 NMR Spectroscopy

^{1}H NMR spectra were acquired in 5 mm NMR tubes at 298 K on Bruker DPX 500 (^{1}H = 500.13 MHz) spectrometers. ^{1}H NMR chemical shifts were internally referenced to $CHCl_3$ (7.26 ppm) for chloroform-d_1. ^{13}C NMR chemical shifts were internally referenced to 77.41 ppm, 77.16 ppm, 76.91 ppm for chloroform-d_1. All data was carried out using XWIN-NMR version 3.6 (Bruker UK Ltd.).

1.2 X-ray Crystallography

All diffraction data were obtained on a Bruker Smart Apex CCD diffractometer equipped with graphite-monochro mated Mo Kα radiation. Absorption corrections were applied using SADABS program. SQUEEZE option was used to remove the non-localized electron density at the final step of structure refinement. The structures were solved by direct methods using SHELXS (TREF) with additional light atoms found by Fourier methods. Complexes were refined against *F*2 using SHELXL, and hydrogen atoms were added at calculated positions and refined riding on their parent atoms. X-ray crystallographic data for **Ir1** are available as Tables S1 and S2 and deposited in the Cambridge Crystallographic Data Centre under the accession numbers CCDC 2106789.

1.3 UV-vis Spectroscopy

The UV-vis spectra of these complexes were recorded by TU-1901 UV spectrophotometer with 1 cm path-length quartz cuvettes (3 mL). Spectra were processed using UV Winlab software. Experiments were carried out at 298 K unless otherwise stated.

1.4 BSA binding experiments

The titration experiments including UV-vis absorption and fluorescence quenching were performed at constant concentration of BSA. A BSA stock solution was prepared in Tris buffer (5 mM Tris–HCl/10 mM NaCl at pH = 7.2) and stored at 277 K. All spectra were recorded after each successive addition of the compounds and incubation at room temperature for 5 min to complete the interaction. In the UV–vis absorption titration experiment, BSA solution (2.5 mL, 1.0×10^{-5} M) was titrated by successive additions of the stock solutions of **Ir1-Ir4** (1.0×10^{-6} M) and the changes in the BSA absorption were recorded after each addition. The fluorescence emission spectra of BSA in the absence and presence of **Ir1-Ir4** were also recorded with excitation at 285 nm. The concentrations of the **Ir1-Ir4** were 0–10.0 μM, and the concentration of BSA was fixed at 10 μM. Synchronous fluorescence spectra of BSA with various concentrations of complexes (0–10.0 μM) were obtained from 240 to 340 nm when $\Delta\lambda$ = 60 nm and from 260 to 360nm when $\Delta\lambda$ = 15 nm.

1.5 Reaction with NADH

The reaction of **Ir1-Ir4** (ca. 1 μM) with NADH (ca. 100 μM) in 20% MeOH/80% H_2O (*v/v*) was monitored by UV-vis at 298 K after various time intervals. TON was calculated from the difference in NADH concentration after 8 h divided by the concentration of iridium catalyst. The concentration of NADH was obtained using the extinction coefficient $\varepsilon_{339} = 6220\ M^{-1}cm^{-1}$.

1.6 Cell Culture

Both human cancer cells (cervical carcinoma HeLa cells and lung cancer A549 cells) were obtained from Shanghai Institute of Biochemistry and Cell Biology (SIBCB) and were grown in Dubelco's Modified Eagle Medium (DMEM). All media were supplemented with 10% fetal bovine serum, and 1% penicillin-streptomycin solution. All cells were grown at 310 K in a humidified incubator under 5% CO_2 atmosphere.

1.7 MTT assay

After plating 5000 cells per well in 96-well plates, the cells were preincubated in drug-free media at 310 K for 24 h before adding different concentrations of the compounds to be tested. In order to prepare the stock solution of the drug, the solid complex was dissolved in DMSO. This stock was further diluted using cell culture medium until working concentrations were achieved. The drug exposure period was 24 h. Subsequently, 15 μL of 5 mg mL^{-1} MTT solution was added to form a purple formazan. Afterwards, 100 μL of dimethyl sulfoxide (DMSO) was transferred into each well to dissolve the purple formazan, and results were measured using a microplate reader (DNM-9606, Perlong Medical, Beijing, China) at an absorbance of 570 nm. Each well was triplicated and each experiment repeated at least three times. IC_{50} values quoted are mean ± SEM.

1.8 Measurement of lipophilicity (log$P_{o/w}$)

The octanol-water partition coefficients ($P_{o/w}$) of complexes were determined using a shake-flask method. Water (50 mL, distilled after milli-Q purification) and 1-octanol (50 mL, vacuum distilled) were shaken together using a laboratory shaker, for 72 h to allow saturation of both phases. Stock solutions of Ir1 and Ir3 (50 μM) were prepared in the aqueous phase and aliquots (5 mL) of each of these stock solutions were then added to an equal volume of the 1-octanol phase. The resultant biphasic solutions were mixed for 2 h and then centrifuged (3000×g, 5 min) to separate the phases. The concentrations of Ir1 and Ir3 in the organic and aqueous phases were then determined using UV-Vis. Log$P_{o/w}$ was defined as the logarithm of the ratio of the concentrations of the compound in the organic and aqueous phases (Values reported are the means of three separate determinations).

1.9 ROS Determination

Flow cytometry analysis of ROS generation in A549 cells caused by exposure to iridium

complexes were carried out using the Reactive Oxygen Species Assay Kit (Beyotime Institute of Biotechnology, Shanghai, China) according to the supplier's instructions. Briefly, 1.5×10^6 A549 cancer cells per well were seeded in a six-well plate. Cells were preincubated in drug-free media at 310 K for 24 h in a 5% CO_2 humidified atmosphere, and then drugs were added at concentrations of $0.25\times IC_{50}$ and $0.5\times IC_{50}$. After 24 h of drug exposure, cells were washed twice with PBS and then incubated with the DCFH-DA probe (10 μM) at 310 K for 30 min, and then washed triple immediately with PBS. The fluorescence intensity was analyzed by flow cytometry (ACEA NovoCyte, Hangzhou, China). Data were processed using NovoExpress™ software.

1.10 Cell Cycle Analysis

The A549 cancer cells at 1.5×10^6 per well were seeded in a six-well plate. Cells were preincubated in drug-free media at 310 K for 24 h, after which **Ir3** were added at concentrations of $0.25\times IC_{50}$, $0.5\times IC_{50}$, $1.0\times IC_{50}$ and $2.0\times IC_{50}$ of **Ir3** against A549 cancer cells. After 24 h of drug exposure, supernatants were removed by suction and cells were washed with PBS. Finally, cells were harvested using trypsin-EDTA and fixed for 24 h using cold 70% ethanol. DNA staining was achieved by suspending the cell pellets in PBS containing propidium iodide (PI) and RNAse. Cell pellets were washed and suspended in PBS before being analyzed in a flow cytometer (ACEA NovoCyte, Hangzhou, China) using excitation of DNA-bound PI at 488 nm, with emission at 585 nm. Data were processed using NovoExpress™ software. The cell cycle distribution is shown as the percentage of cells containing G_0/G_1, S and G_2/M DNA as identified by propidium iodide staining.

1.11 Induction of Apoptosis

Flow cytometry analysis of apoptotic populations of the cells caused by exposure to **Ir3** were carried out using the Annexin V-FITC Apoptosis Detection Kit (Beyotime Institute of Biotechnology, China) according to the supplier's instructions. Briefly, A549 cancer cells (1.5×10^6/2 mL per well) were seeded in a six-well plate. Cells were preincubated in drug-free media at 310 K for 24 h, after which **Ir3** was added at concentrations of $0.5\times IC_{50}$, $1.0\times IC_{50}$, $2.0\times IC_{50}$ and $3.0\times IC_{50}$ of **Ir3** against A549 cancer cells. After 24 h of drug exposure, cells were collected, washed once with PBS, and suspended in 195 μL of annexin V-FITC binding buffer which was then added to 5 μL of annexin V-FITC and 10 μL of PI, and then incubated at room temperature in the dark for 15 min. Subsequently, the buffer placed in an ice bath in the dark. The samples were analyzed by a flow cytometer (ACEA NovoCyte, Hangzhou, China).

1.12 Mitochondrial Membrane Assay

Analysis of the changes of mitochondrial potential in cells after exposure to iridium complexes

was carried out using the mitochondrial membrane potential assay kit with JC-1 (Beyotime Institute of Biotechnology, Shanghai, China) according to the manufacturer's instructions. Briefly, 1.5×10^6 A549 cancer cells were seeded in six-well plates left to incubate for 24 h in drug-free medium at 310 K in a humidified atmosphere. Drug solutions, with the concentration changed from $0.5\times IC_{50}$ to $2.0\times IC_{50}$ of **Ir3** against A549 cancer cells, were added in triplicate, and the cells were left to incubate for a further 24 h under similar conditions. Supernatants were removed by suction, and each well was washed with PBS before detaching the cells using trypsin-EDTA. Staining of the samples was done in flow cytometry tubes protected from light, incubating for 30 min at ambient temperature. The samples were immediately analyzed by a flow cytometer (ACEA NovoCyte, Hangzhou, China). For positive controls, the cells were exposed to carbonyl cyanide 3-chlorophenylhydrazone, CCCP (5 μM), for 20 min. Data were processed using NovoExpress™ software.

1.13 Cellular localization assay

Two Photon Laser Scanning Microscope (*/LSM/880NLO) is produced at Carl Zeiss AG, Germany. LTDR (Life Technologies, USA), MTDR (Life Technologies, USA), CCCP (Sigma Aldrich, USA), chloroquine (Sigma Aldrich, USA) were used as received. A549 cells were seeded into 35 mm dishes (Greiner, Germany) for confocal microscopy. After cultured overnight, the cells were incubated with **Ir3** ($1.0\times IC_{50}$) for 1 h. The treated cells were observed immediately under a confocal microscope with excitation at 405 nm. For colocalization studies, the cells were incubated with complexes ($1.0\times IC_{50}$) for 1 h. Subsequently, the medium was replaced with staining medium containing MTDR/LDTR and stained for another 20 min and 1 h. The cells were washed twice with PBS, and then viewed immediately under a confocal microscope. Investigation of drug entry pattern: Cells were incubated with complexes ($1.0\times IC_{50}$) for 1 h, after which media was replaced with staining medium containing CCCP (10 μM, 1 h) chloroquine (50 μM, 1 h) and re-stained for 15 min. The cells were washed twice with PBS, and then viewed immediately under a confocal microscope.

1.14 Assay for the lysosomal membrane permeabilization (AO assay)

A549 cells seeded into six-well plate (Corning) were exposed to **Ir3** at the indicated concentrations for 12 h. The cells were then washed twice with PBS and incubated with AO (5 μM) at 310 K for 15 min. The cells were washed twice with PBS and visualized by confocal microscopy (LSM/880NLO). Emission was collected at 510±20 nm (green) and 625±20 nm (red) upon excitation at 488 nm.

1.15 Assay for the Inhibition of cell migration

A549 cells (1,500,000 per well) were seeded in 2000 μL media in 6-well plates and allowed

to attach and grow to form a confluent monolayer. Each well of the plates was marked with a horizontal line passing through the center of bottom in advance. Wounds were created perpendicular to the lines by 10 μL tips, and unattached cells were removed by washing with PBS (pH = 7.4). **Ir1** and **Ir3** in DMEM with 1% FBS was added and cells incubated at 310 K under 5% CO_2 for imaging. DMEM with 1% FBS was used to suppress cell proliferation. Images were captured at 0 and 24 h at the same position of each well. Experiments were repeated for at least three times.

1.16 Experimental

Synthesis of [(η^5-C_5Me_5)$IrCl_2$]$_2$ (Dimer 1) and [(η^5-$C_5Me_4C_6H_5$)$IrCl_2$]$_2$ (Dimer 2)

Dimers were prepared according to literature methods[1].

Dimer 1: Yield: 0.40 g (65%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.60 (s, *J* = 1.4 Hz, 30H).

Dimer 2: Yield: 0.37 g (58.5%). ^{1}H NMR (500 MHz, $CDCl_3$): δ 7.58 (m, 4H), 7.35 (m, 6H), 1.72 (s, 12H), 1.63 (s, 12H)

Synthesis of Schiff base pro-ligands (L1 and L2)

The general process is as follows: Amino-substitued *N*-phenylcarbazole/triphenylamine (10 mmol) was dissolved in ethanol (50 mL). Salicylaldehyde (10 mmol) was added dropwise under stirring, 3 drops formic acid added and a solid precipitate was obtained. The mixture was heated under reflux for 5 h, and then cooled to room temperature. Pressure filtration, solid was recrystallized from ethanol to give products. The data were as follows:

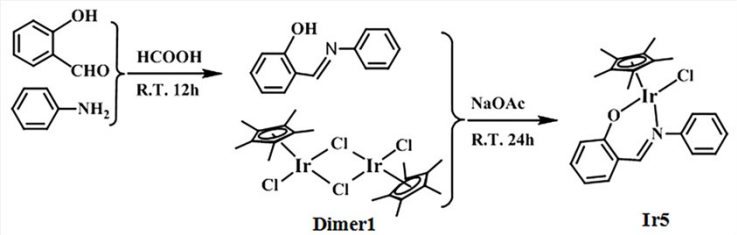
L1: ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.15 (s, 1H), 8.73 (s, 1H), 8.15 (d, *J* = 7.8 Hz, 2H), 7.62 (d, *J* = 8.4 Hz, 2H), 7.51 (d, *J* = 8.5 Hz, 2H), 7.43 (d, *J* = 4.0 Hz, 5H), 7.32 – 7.28 (m, 2H), 7.25 (s, 1H), 7.07 (d, *J* = 8.3 Hz, 1H), 6.98 (t, *J* = 7.4 Hz, 1H). ESI-MS (*m/z*): calcd for $C_{25}H_{18}N_2O$: 362.1 $[M+H]^+$, Found 363.2.

L2: ^{1}H NMR (500 MHz, $CDCl_3$) δ 13.39 (s, 1H), 11.39 (s, 1H), 8.72 (s, 1H), 8.63 (s, 1H), 7.41 – 7.34 (m, 4H), 7.28 (d, *J* = 7.8 Hz, 2H), 7.21 (d, *J* = 8.6 Hz, 2H), 7.11 (d, *J* = 7.6 Hz, 4H), 7.04 (d, *J* = 7.5 Hz, 2H), 6.95 (dd, *J* = 13.9, 7.3 Hz, 2H). ESI-MS (*m/z*): calcd for $C_{25}H_{20}N_2O$: 364.2 $[M+H]^+$, Found 365.2.

Synthesis of the [(η^5-Cp^x)Ir(O^N)Cl] (Ir5)

To a 200 mL round bottom flask, 0.50 g (4.09 mmol) of salicylaldehyde and 0.38 g (4.09 mmol) of aniline were added, respectively. To the above flask, 40 ml of anhydrous methanol was added and added dropwise, 1 d formic acid as a catalyst. The mixed system was stirred and refluxed at 70 ℃ for about 36 h until the reaction was complete. Then the above products (0.024 g, 0.12 mmol) reacted with **Dimer 1** (0.050 g, 0.06 mmol) and sodium acetate (0.033 g, 0.40 mmol)

in nitrogen, and finally the control compound was obtained, Scheme S1. Yield: 0.028 g (83%). ^{1}H NMR (500 MHz, CDCl3): δ 8.02 (s, 1H), 7.68 (d, *J* = 7.9 Hz, 2H), 7.36 (dt, *J* = 20.3, 7.7 Hz, 4H), 7.11 (d, *J* = 7.8 Hz, 1H), 6.97 (d, *J* = 8.6 Hz, 1H), 6.45 (t, *J* = 7.3 Hz, 1H), 1.32 (s, 15H). ESI-MS (*m/z*): Calcd for $C_{23}H_{25}ONIr$: 523.6; Found: 524.2 $[M\text{-}Cl]^+$.

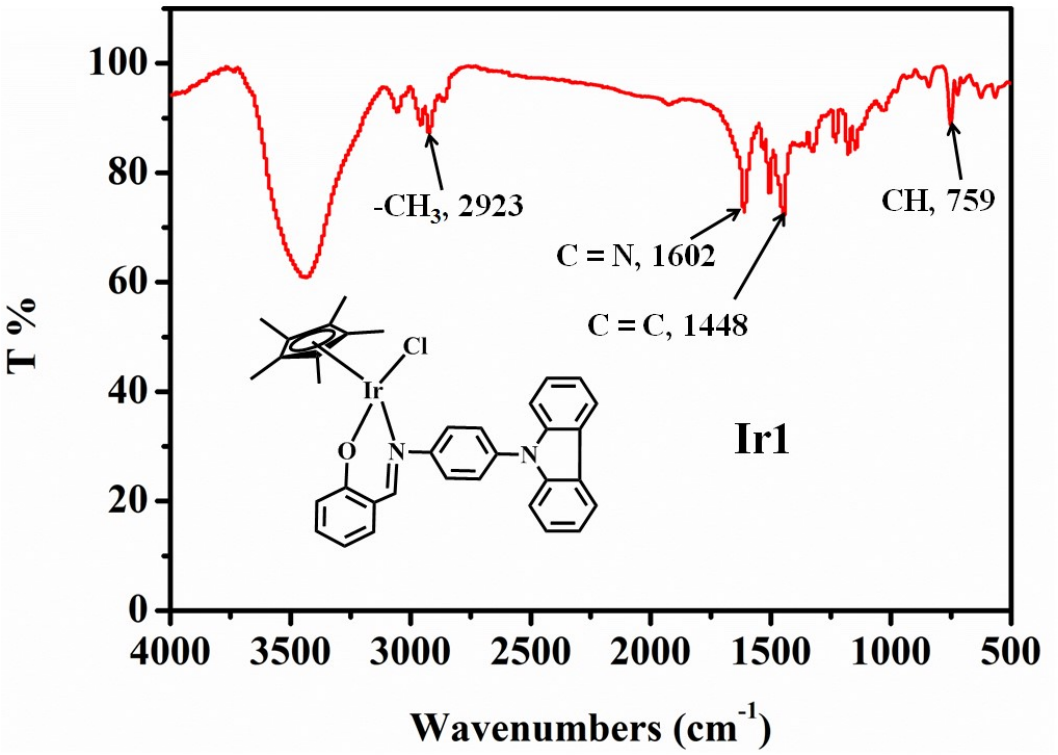


Scheme S1. Synthesis process of **Ir5**.

Notes and Reference

[1] Xiangdong He, Meng Tian, Xicheng Liu, Yanhua Tang, Chang fang Shao, Peiwei Gong, Jinfeng Liu, Shumiao Zhang, Lihua Guo, Zhe Liu. *Chem. Asian. J.* **2018**, 13, 1500-1509.

2 Figures


T %
100
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60
40
20
0
4000
3500
3000
2500
2000
1500
1000
500
Wavenumbers (cm-1)
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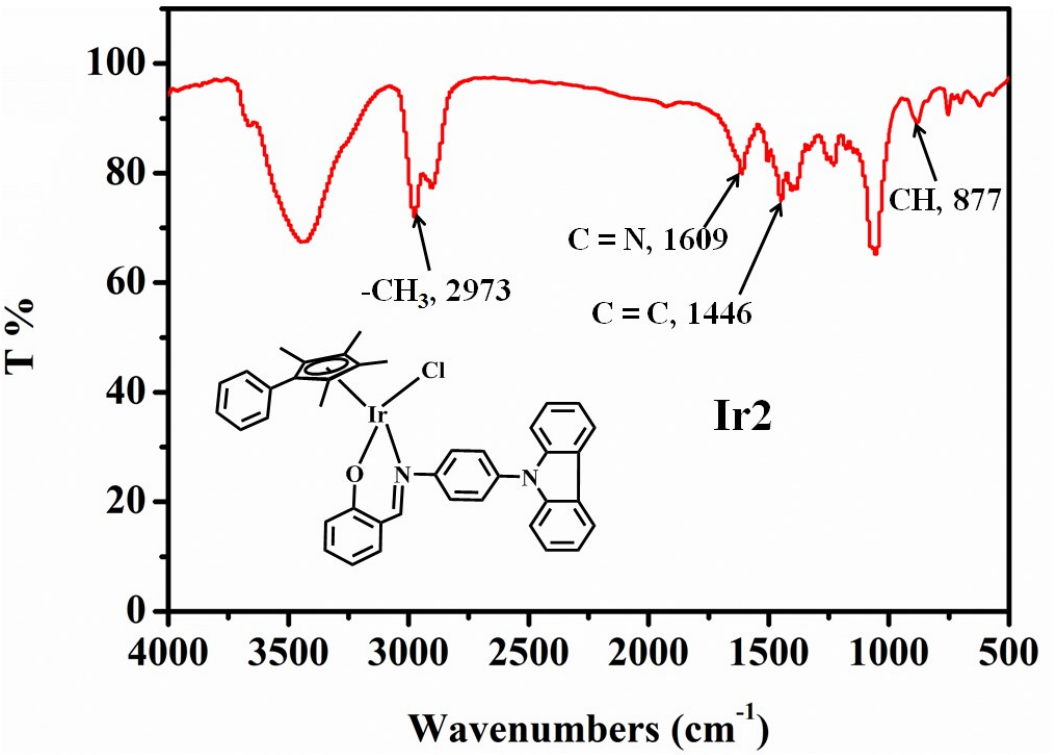
C = C, 1448
CH, 759
Cl
Ir
O
N
N
Ir1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Ir
O
N
N
Ir2

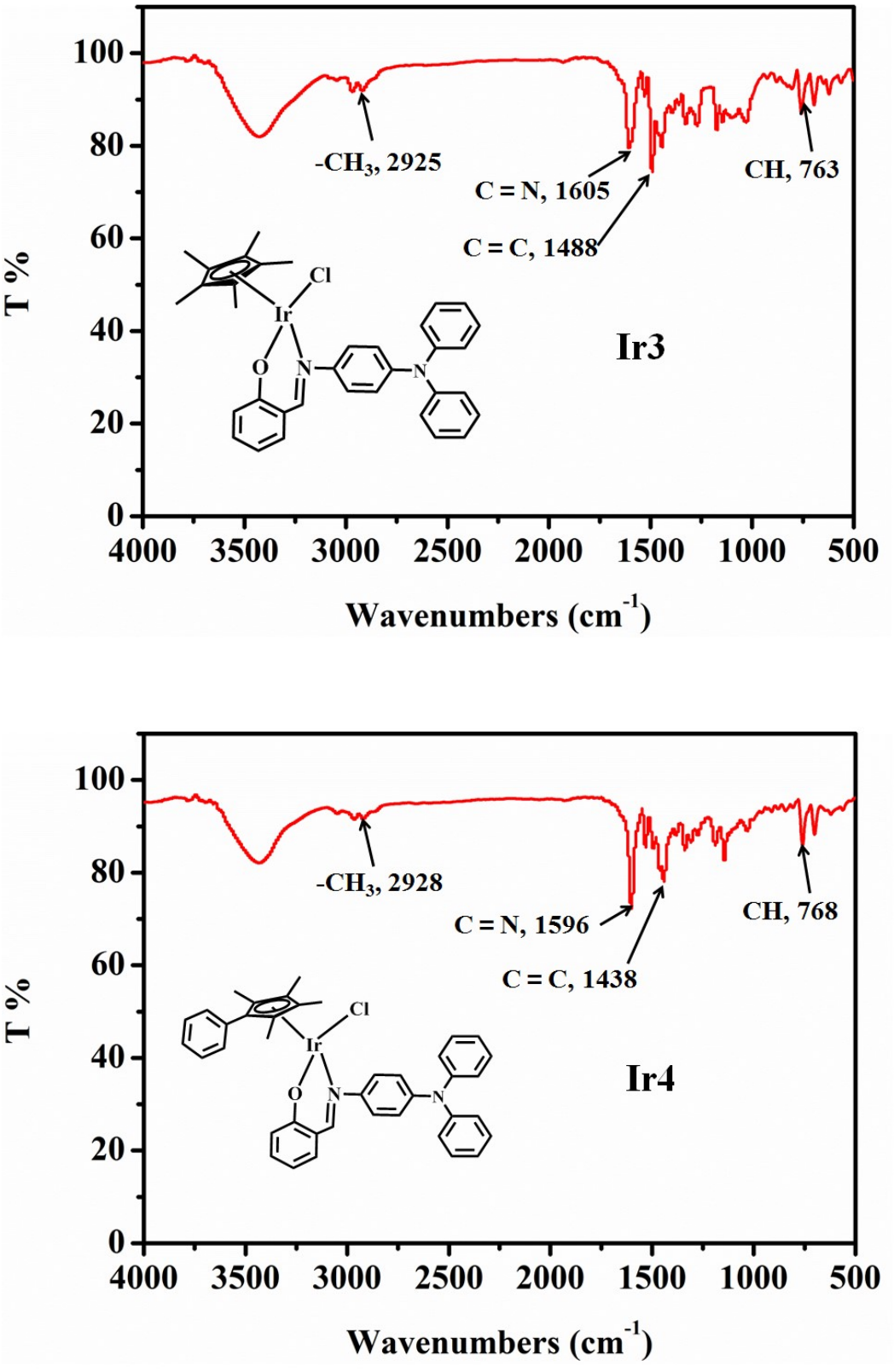
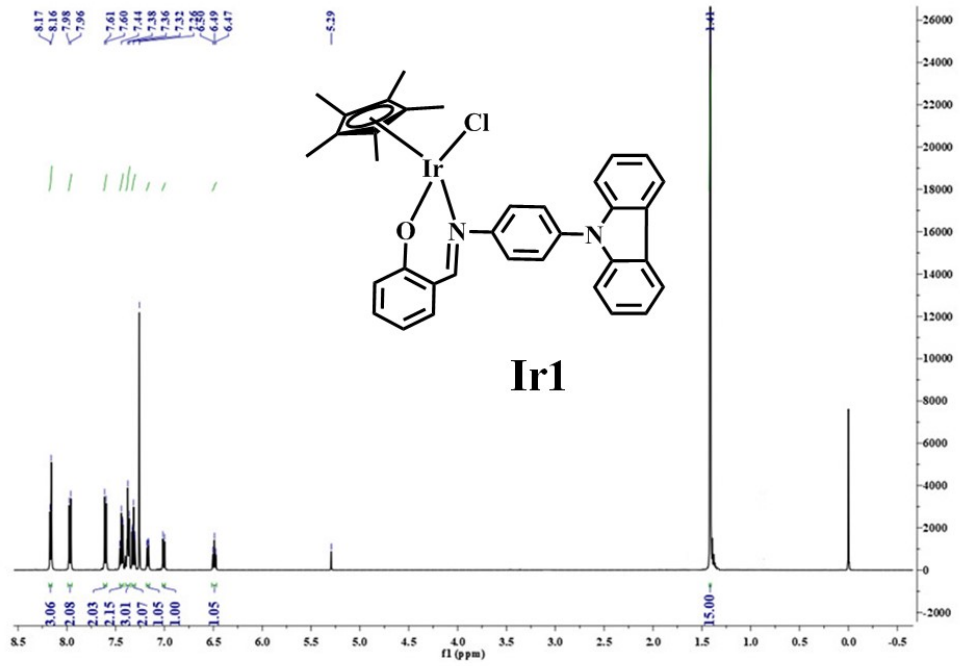
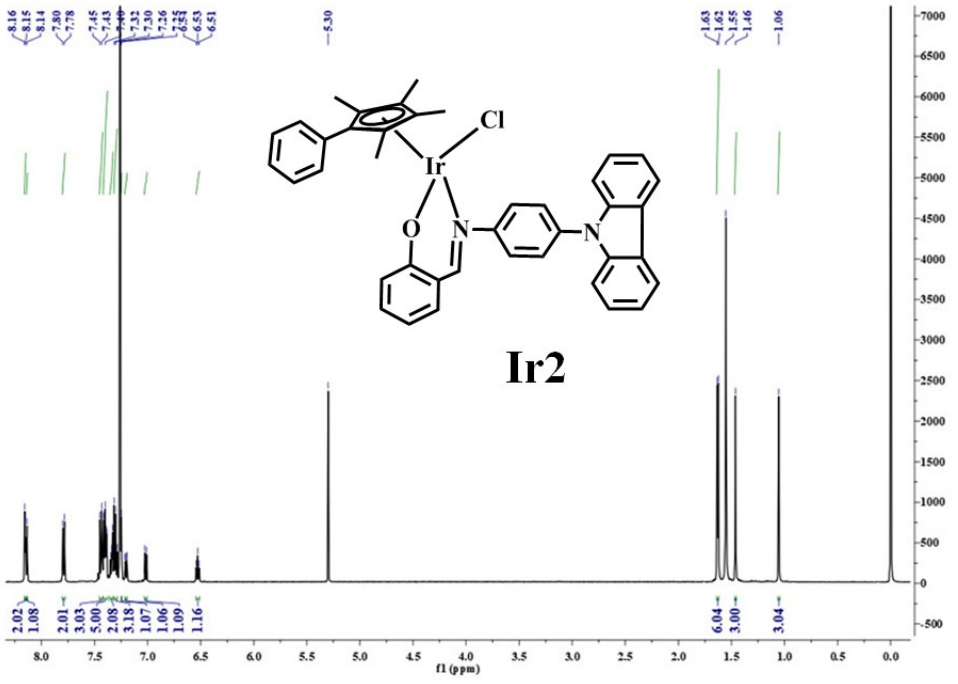


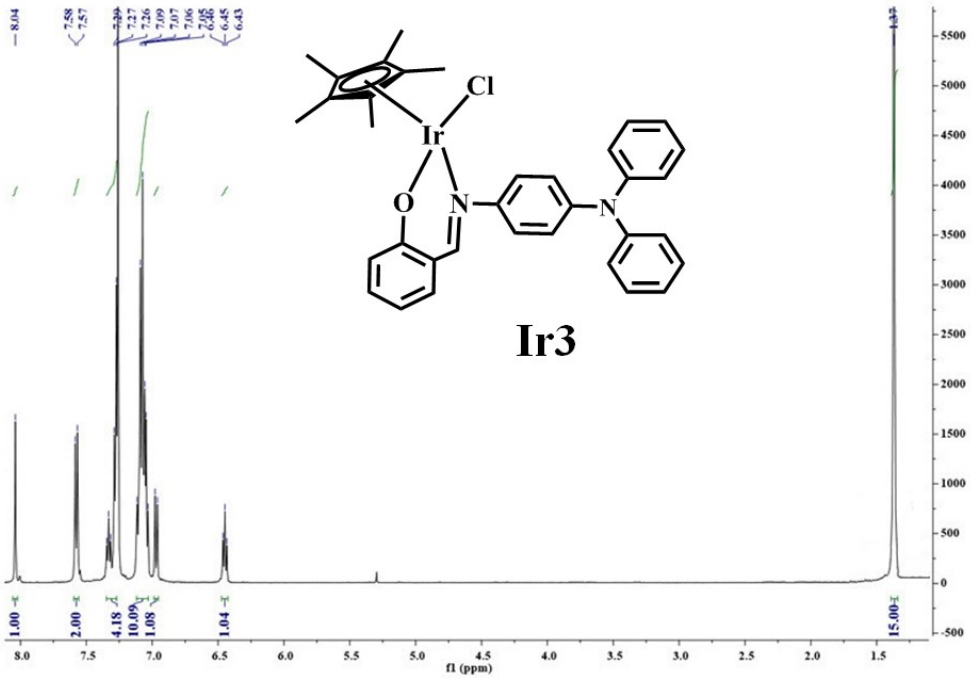
Figure S1 FT-IR spectra of **Ir1-Ir4.**



Ir1



Ir2



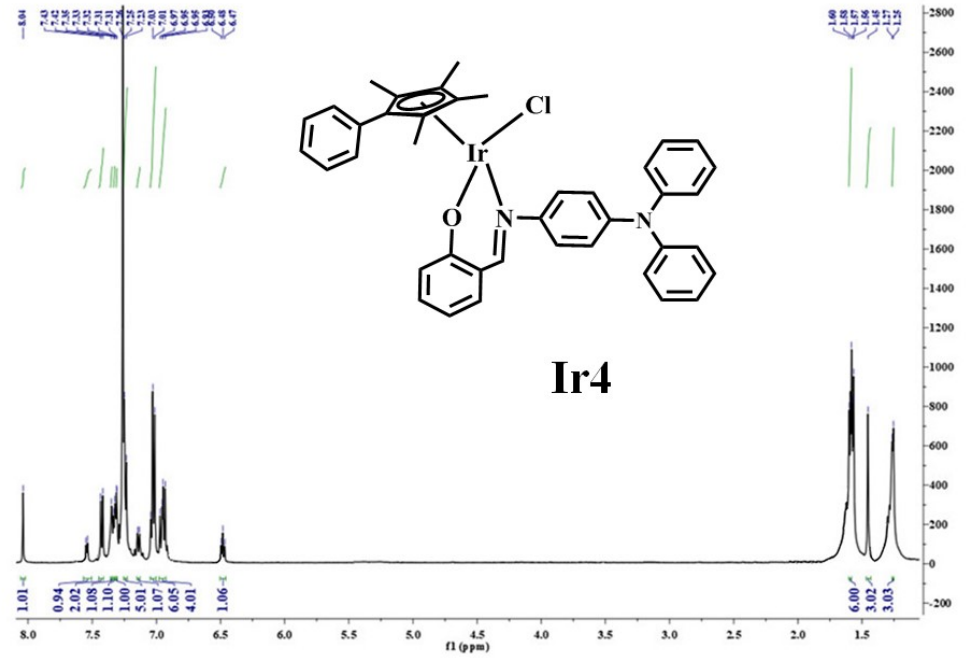
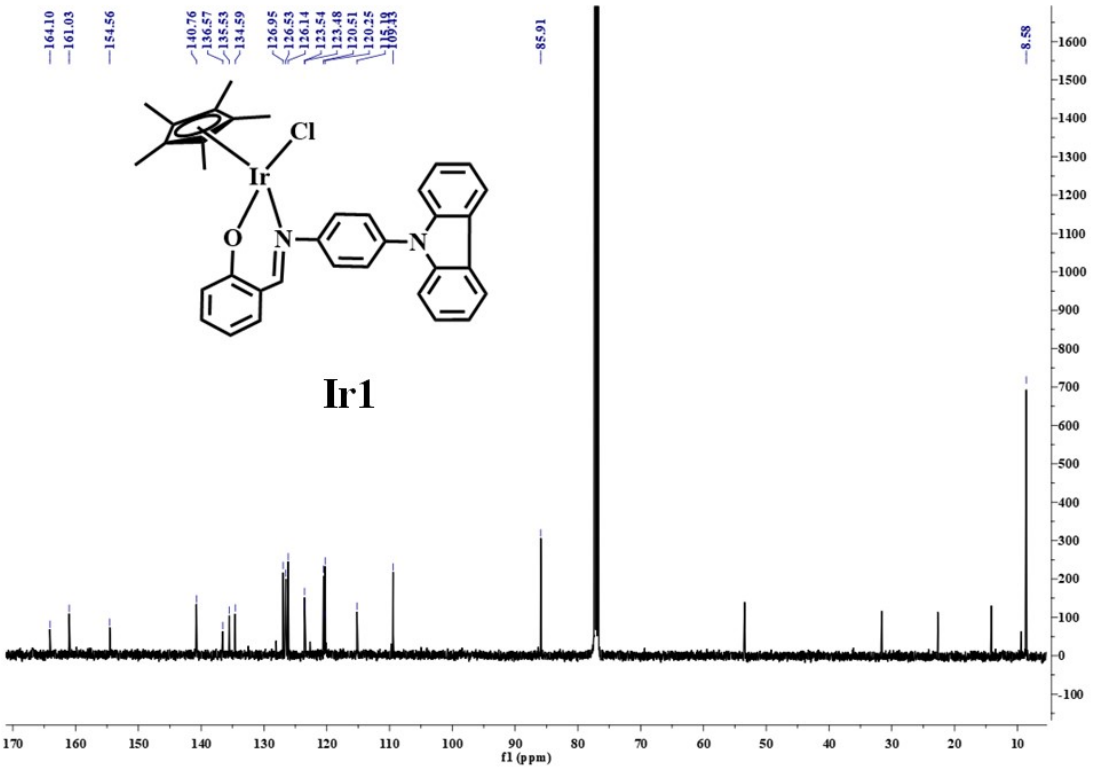


Figure S2 ^{1}H NMR (500 MHz) of **Ir1-Ir4.**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161.03
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140.76
136.57
135.53
134.59
126.95
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126.14
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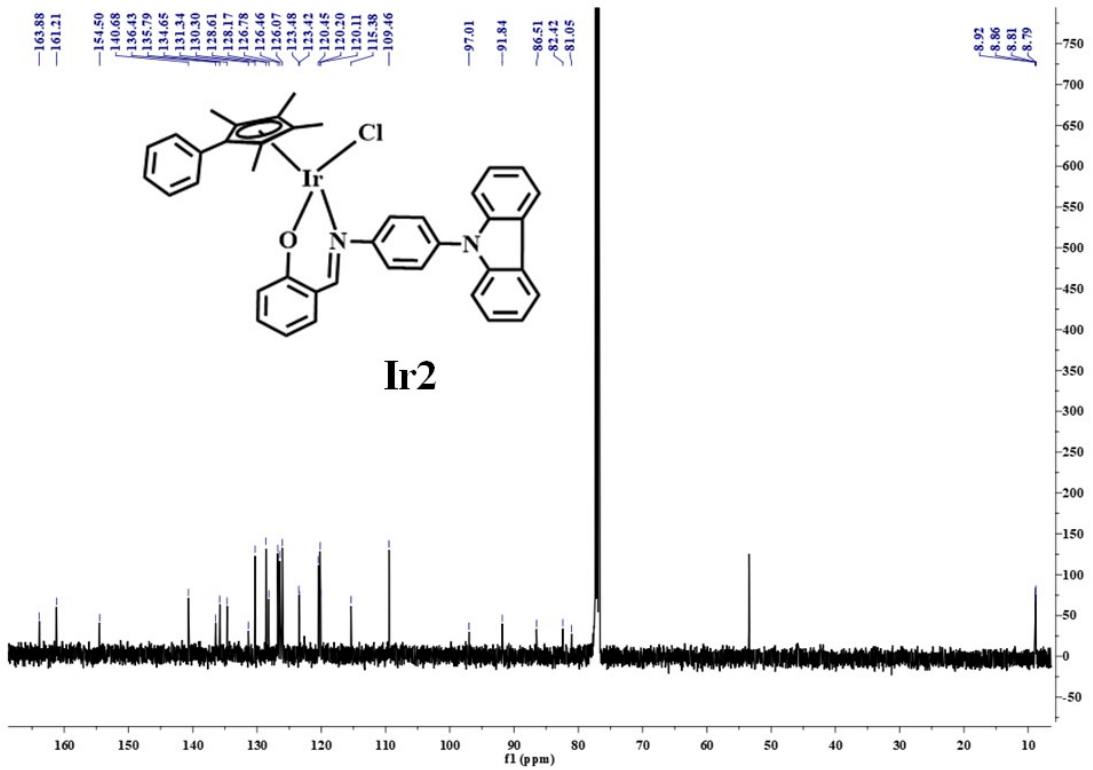
Cl
Ir
O
N
N
Ir1
f1 (ppm)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126.46
126.07
123.48
123.42
120.45
120.20
120.11
115.38
109.46
97.01
91.84
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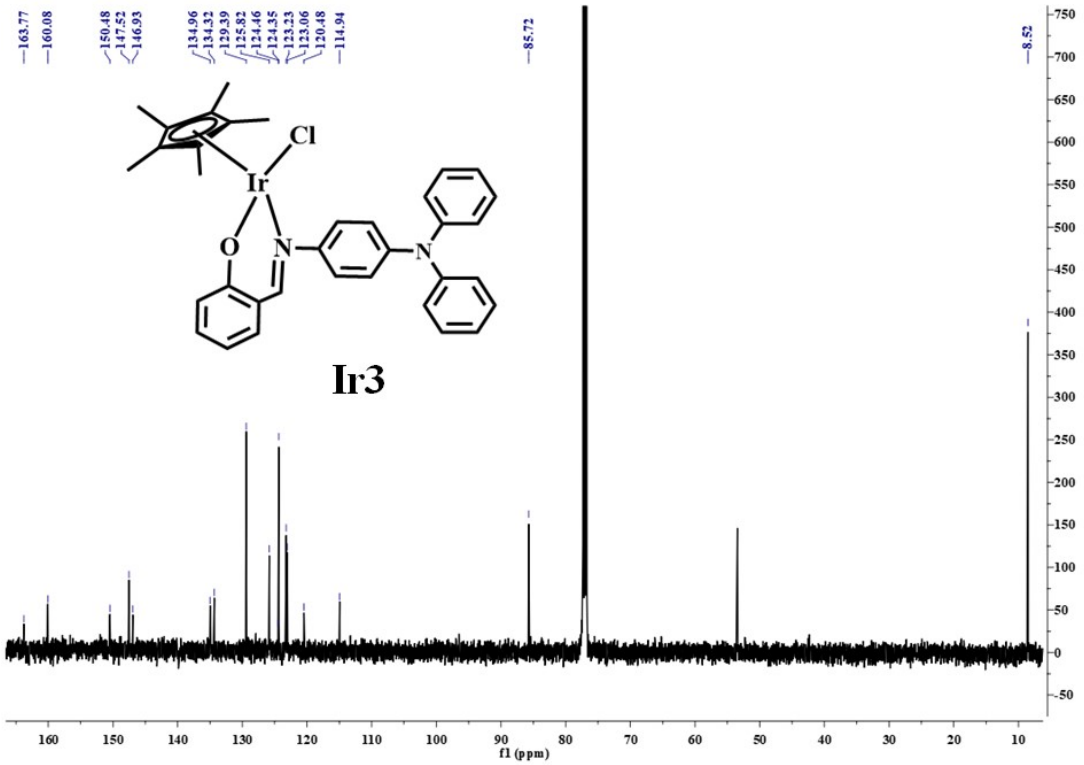
8.79
Cl
Ir
O
N
N
Ir2
f1 (ppm)



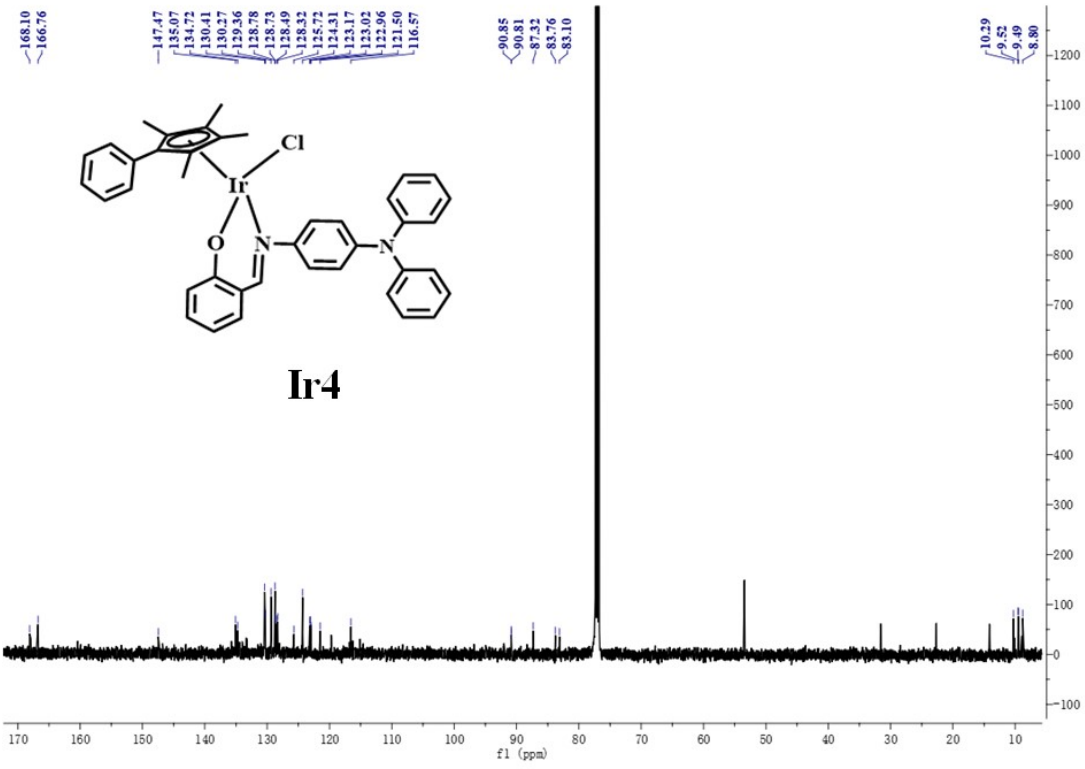
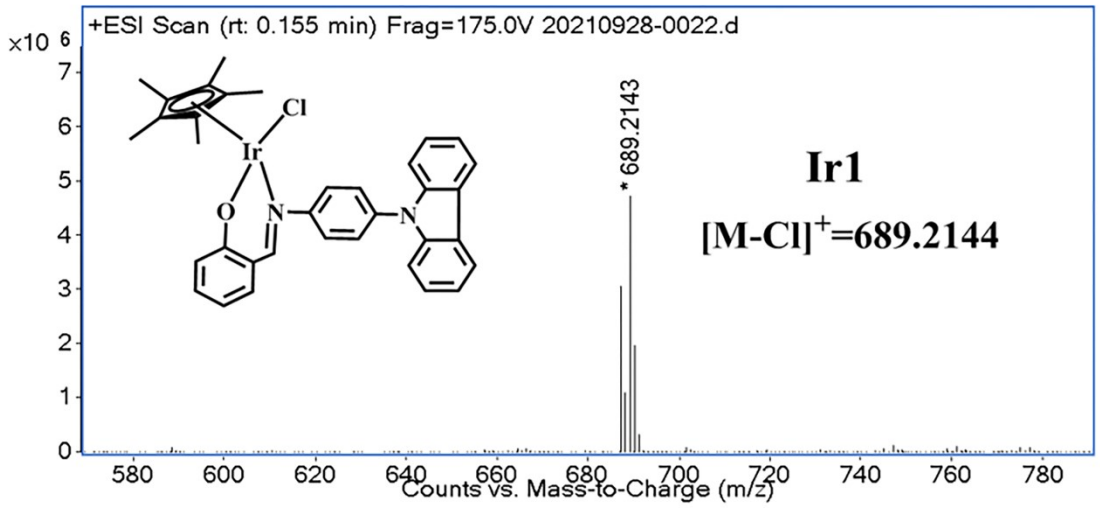


Figure S3 ^{13}C NMR (126 MHz) of **Ir1-Ir4**.


+ESI Scan (rt: 0.155 min) Frag=175.0V 20210928-0022.d
x10 6
Cl
Ir
O
N
N
* 689.2143
Ir1
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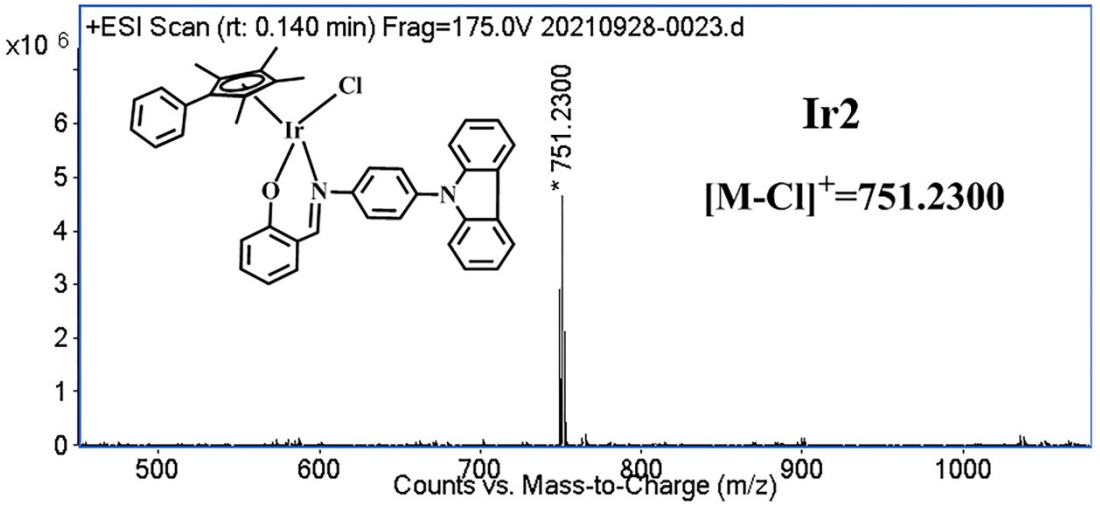
Counts vs. Mass-to-Charge (m/z)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x10 6
Cl
Ir
O
N
N
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Ir2
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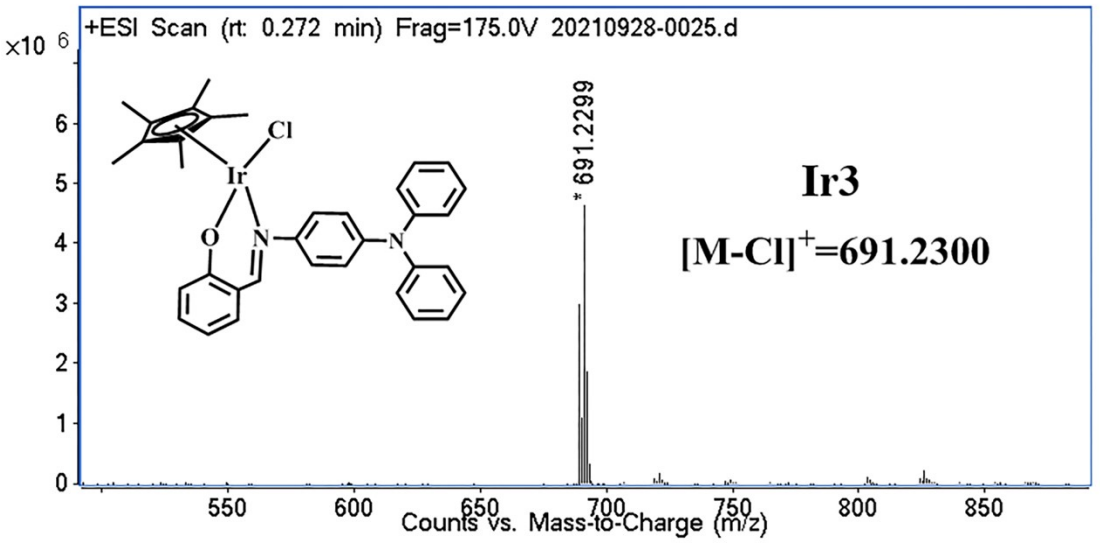
Counts vs. Mass-to-Charge (m/z)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Cl
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O
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N
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Counts vs. Mass-to-Charge (m/z)

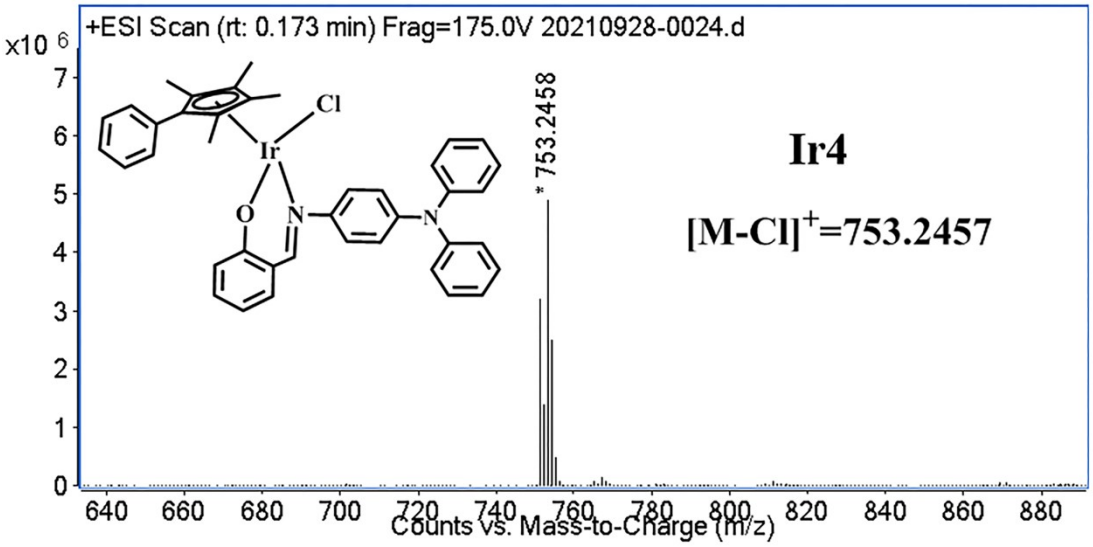
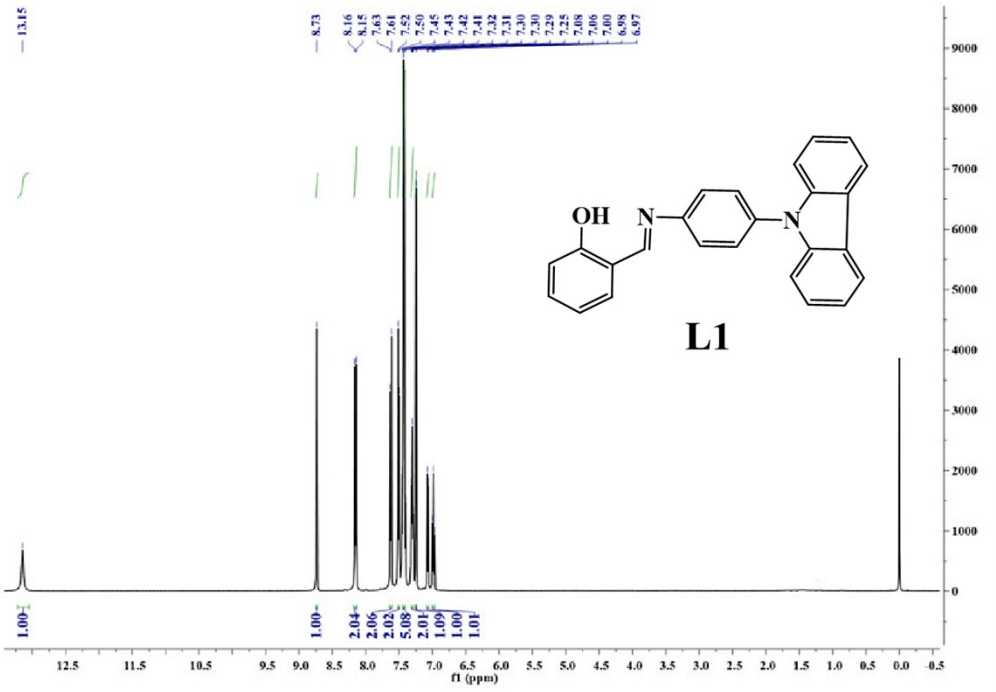


Figure S4 The High resolution mass spectrometry of **Ir1-Ir4**.



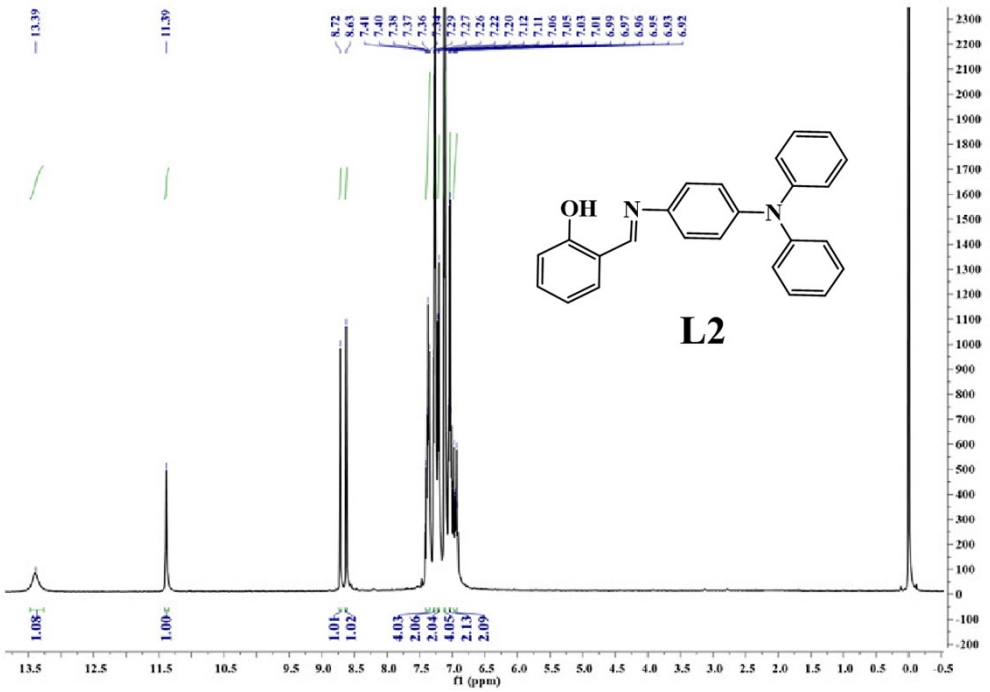
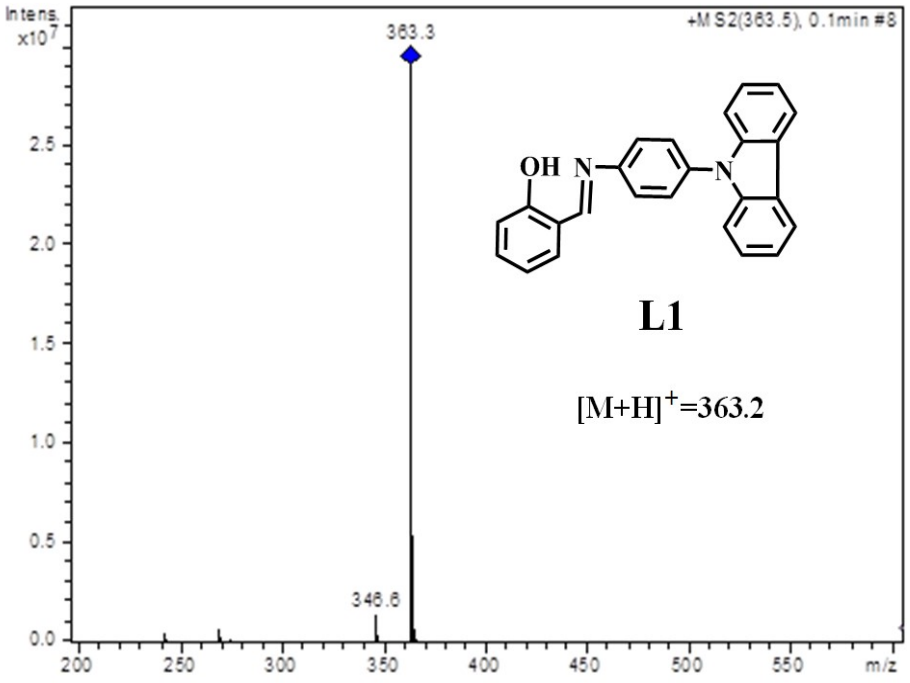


Figure S5 The ^{1}H NMR (500 MHz) of chelating ligands (**L1-L2).**



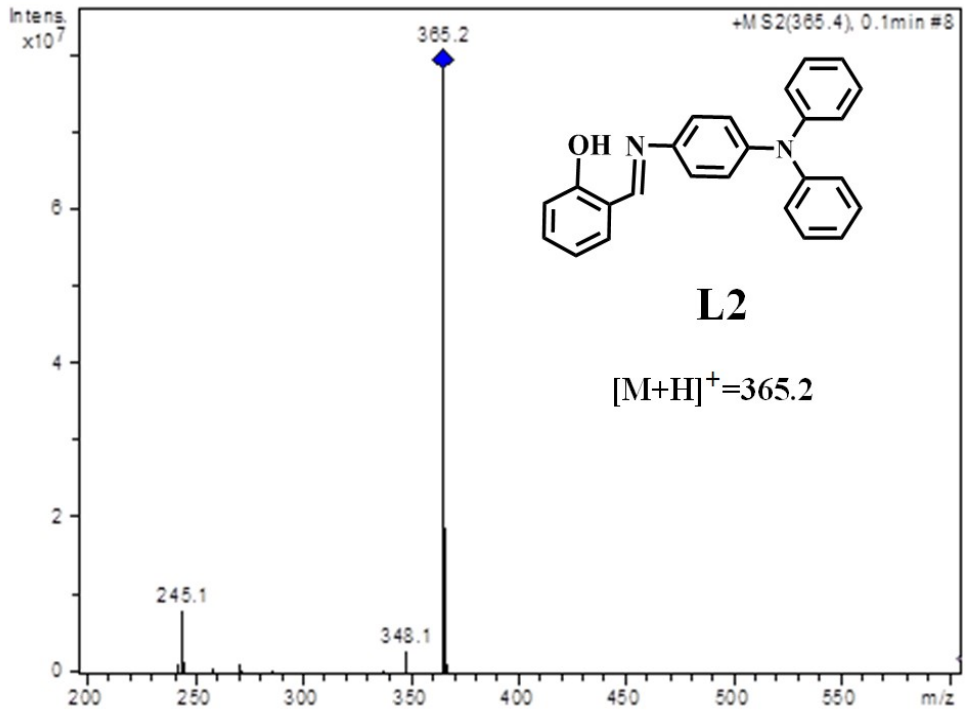


Figure S6 Mass spectra of Schiff base pro-ligands (**L1-L2)**.

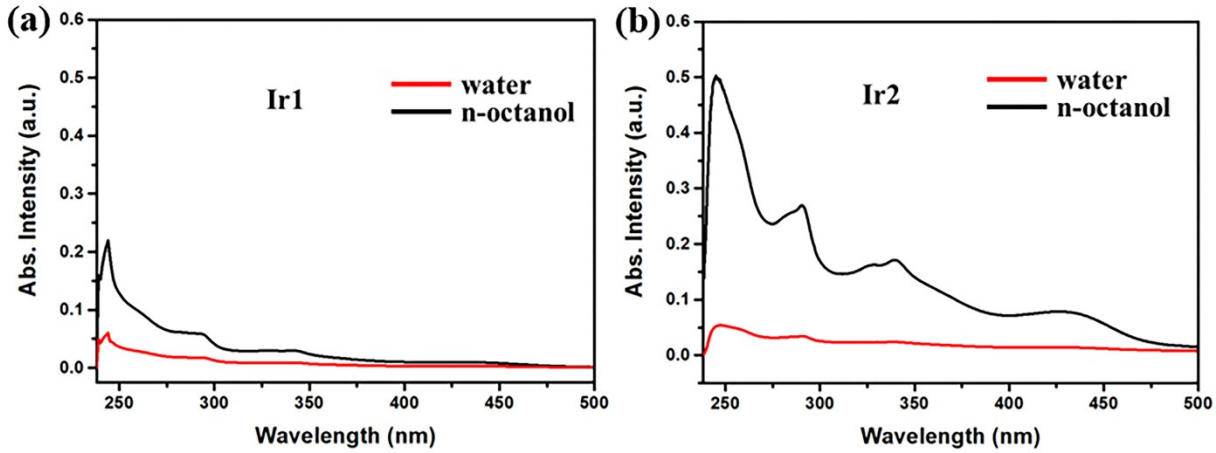


Figure S7 UV-vis absorption spectra of **Ir1** (a) and **Ir2** (b) in water and *n*-octanol.

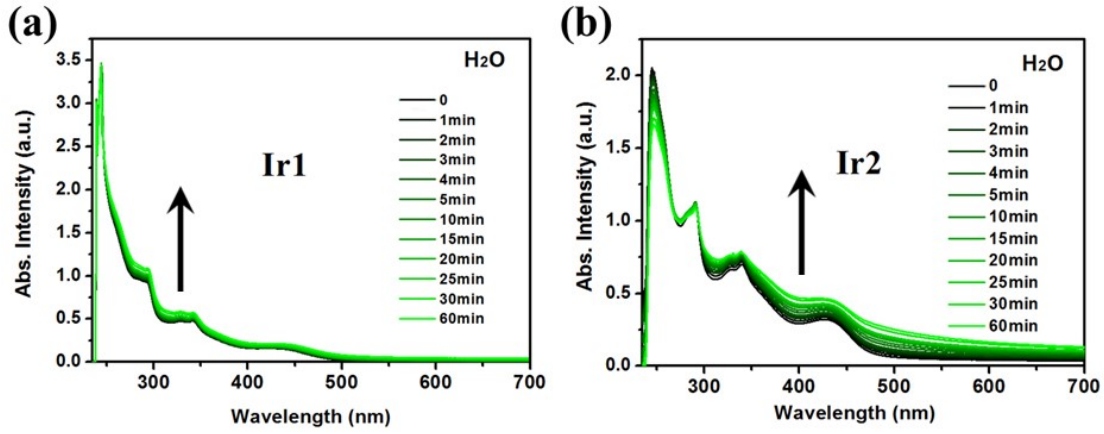


Figure S8 Time-dependant UV-vis absorption spectra of **Ir1** (a) and **Ir2** (b) in 20% DMSO/80%

H_2O (*v/v*) solution at 298 K over 1 h**.** The arrows show the intensity changes with the increase of complexes.

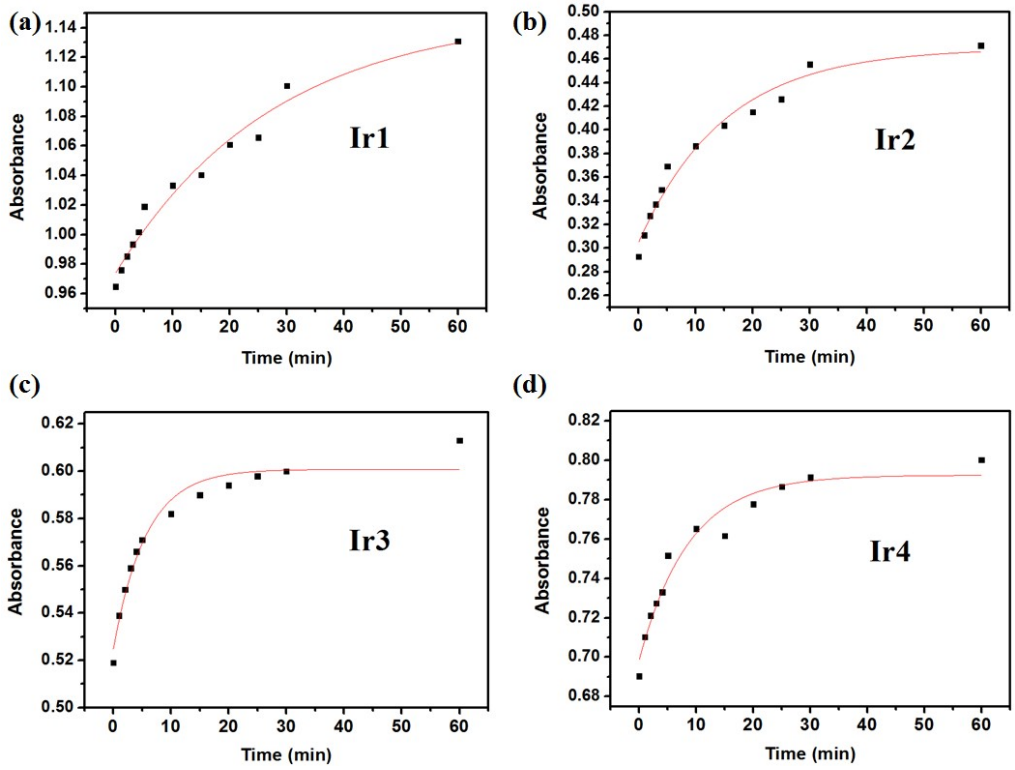


Figure S9 Time dependence of hydrolysis of **Ir1** (a) **Ir2** (b) **Ir3** (c) and **Ir4** (d) based on UV-vis spectra by measuring the absorption difference in 283 nm, 398 nm, 350 nm and 272 nm, respectively.

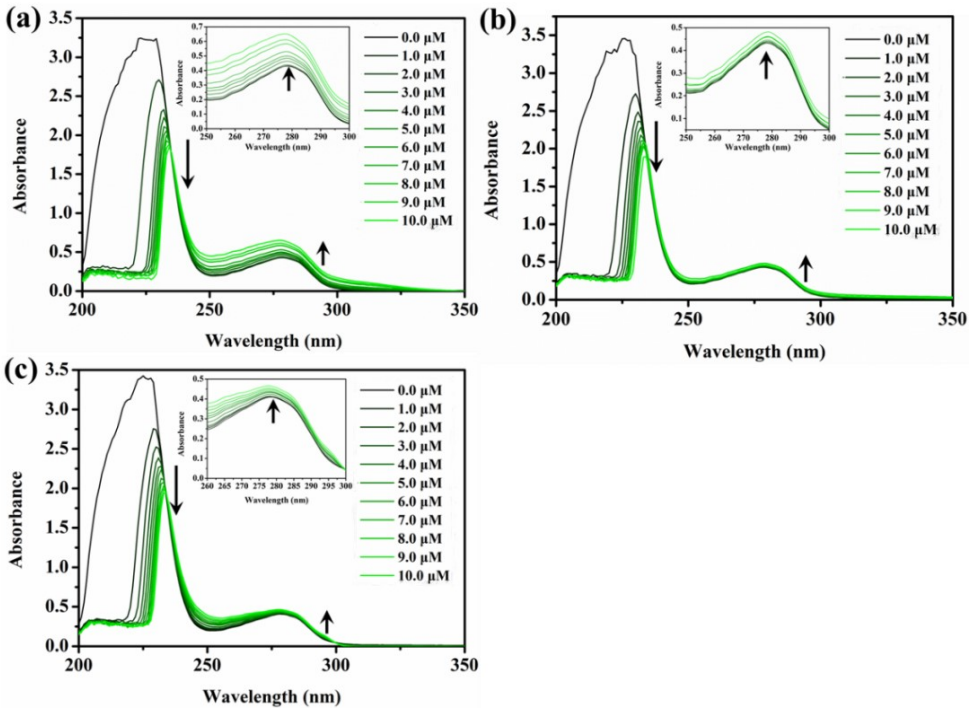


Figure S10 UV-vis spectra of BSA (10.0 μM) in 5 mM Tris-HCl/10 mM NaCl buffer solution (pH: 7.2) upon addition of the **Ir1** (a), **Ir2** (b) and **Ir4** (c) (0.0-10.0 μM). The arrows show the

intensity changes with the increase of complexes.

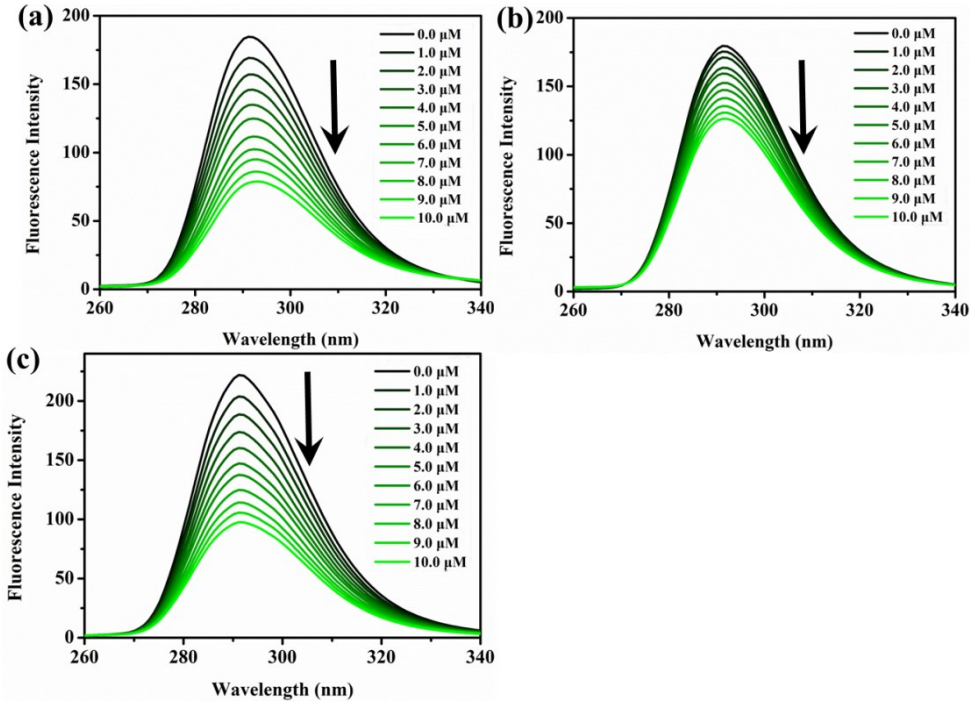


Figure S11 Synchronous spectra of BSA (10.0 μM, 50.0 mM Tris-HCl, 50.0 mM NaCl, pH = 7.2) in the presence of increasing amounts of **Ir1** (a), **Ir2** (b) and **Ir4** (c) (0.0-10.0 μM) with a wavelength difference of $\Delta\lambda$ = 15 nm. The arrows show the intensity changes with the increase of complexes.

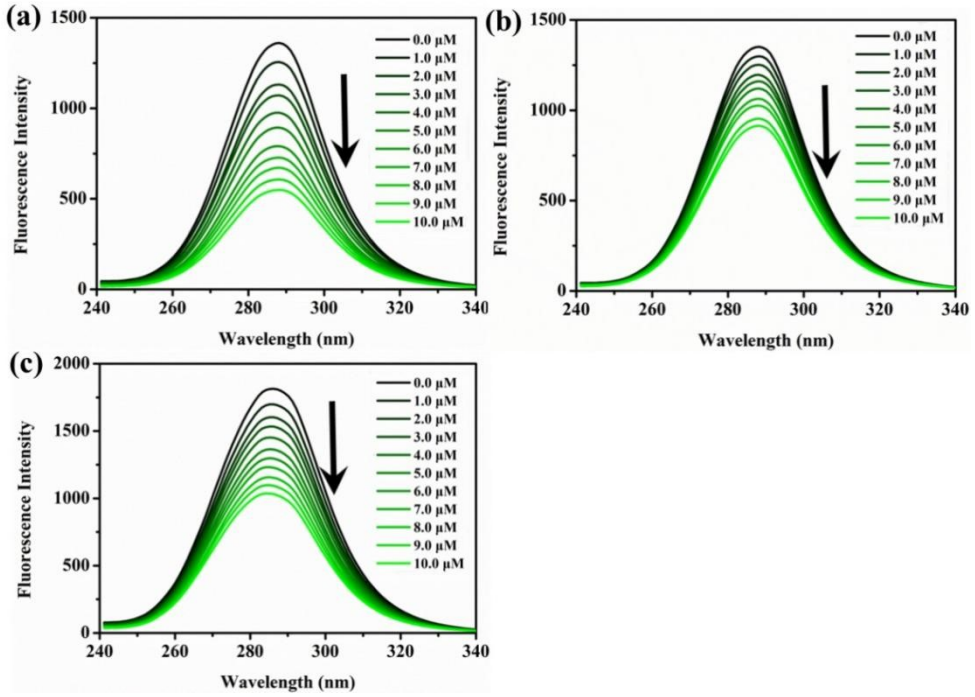


Figure S12 Synchronous spectra of BSA (10.0 μM, 50.0 mM Tris-HCl, 50.0 mM NaCl, pH = 7.2) in the presence of increasing amounts of **Ir1** (a), **Ir2** (b) and **Ir4** (c) (0.0-10.0 μM) with a wavelength difference of $\Delta\lambda$ = 60 nm. The arrows show the intensity changes with the increase of complexes.

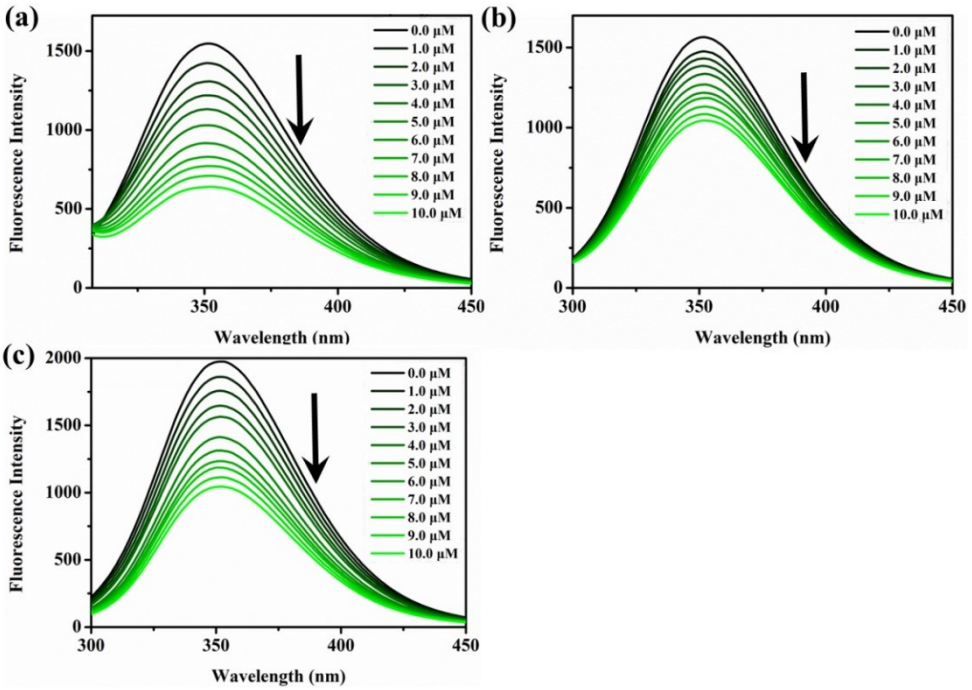


Figure S13 Fluorescence spectra of BSA (10.0 μM; λ_{ex} = 280 nm; λ_{em} = 350 nm) in the absence and presence of the **Ir1** (a), **Ir2** (b) and **Ir4** (c) (0-10.0 μM). The arrows show the intensity changes with the increase of complexes.

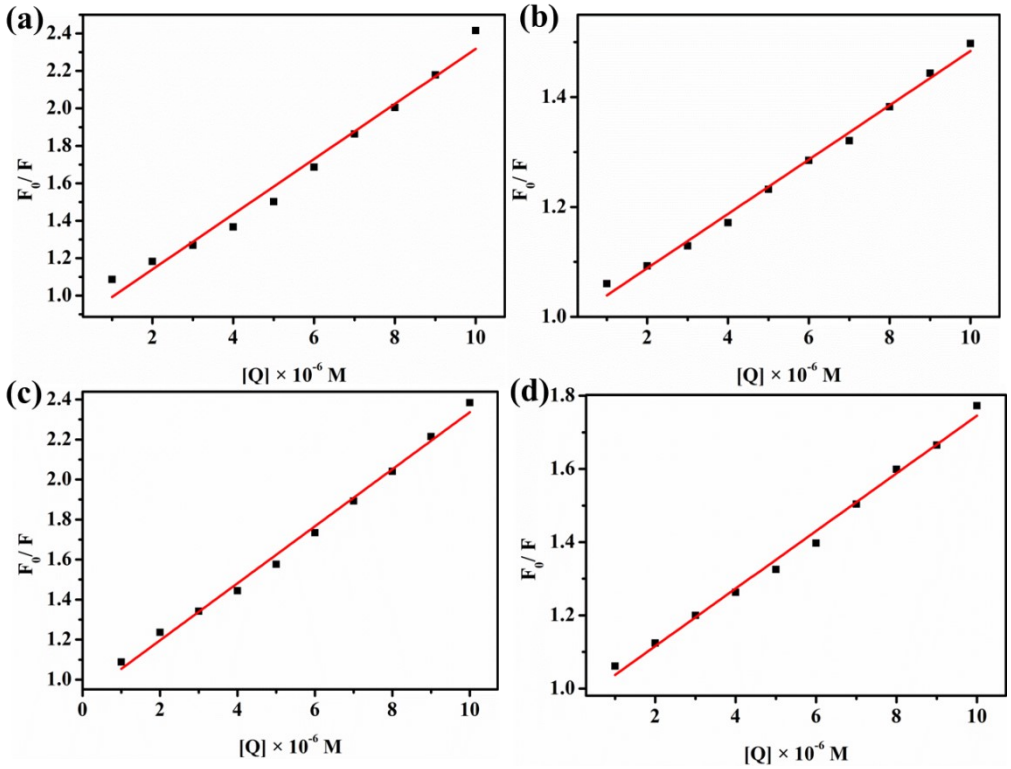


Figure S14 Stern–Volmer plots of F_0/F against the concentration of **Ir1** (a), **Ir2** (b), **Ir3** (c) and **Ir4** (d) (0-10.0 μM).

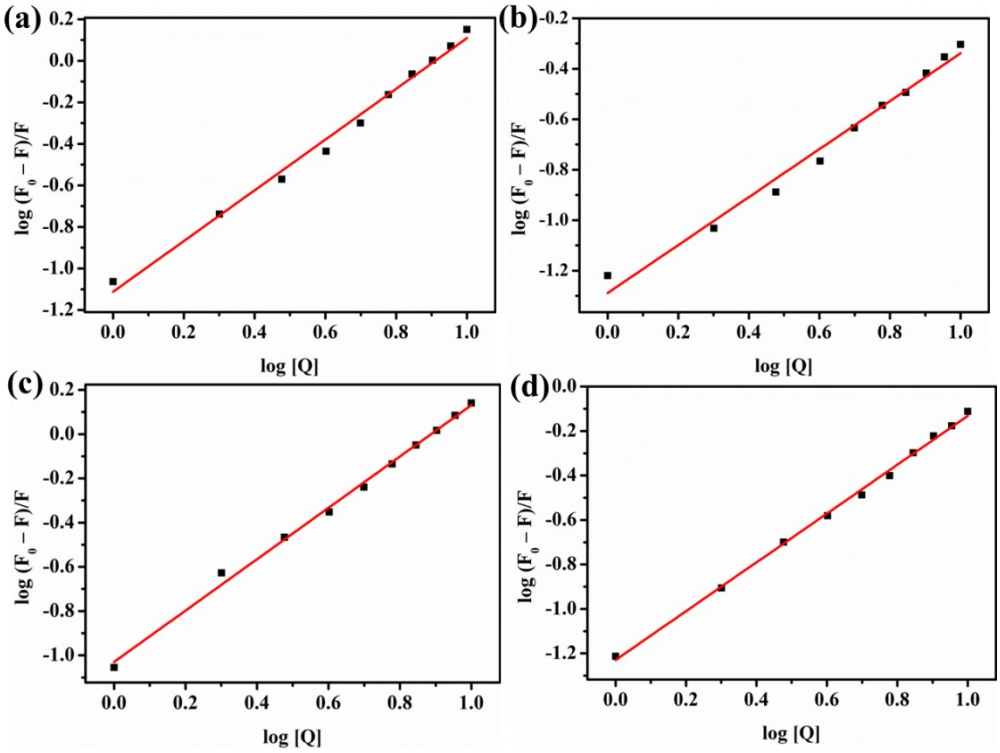


Figure S15 Plots of log [(F_0- F)/F] *vs* log [Q] for the interaction of BSA with **Ir1** (a), **Ir2** (b), **Ir3** (c) and **Ir4** (d) (0-10.0 μM).

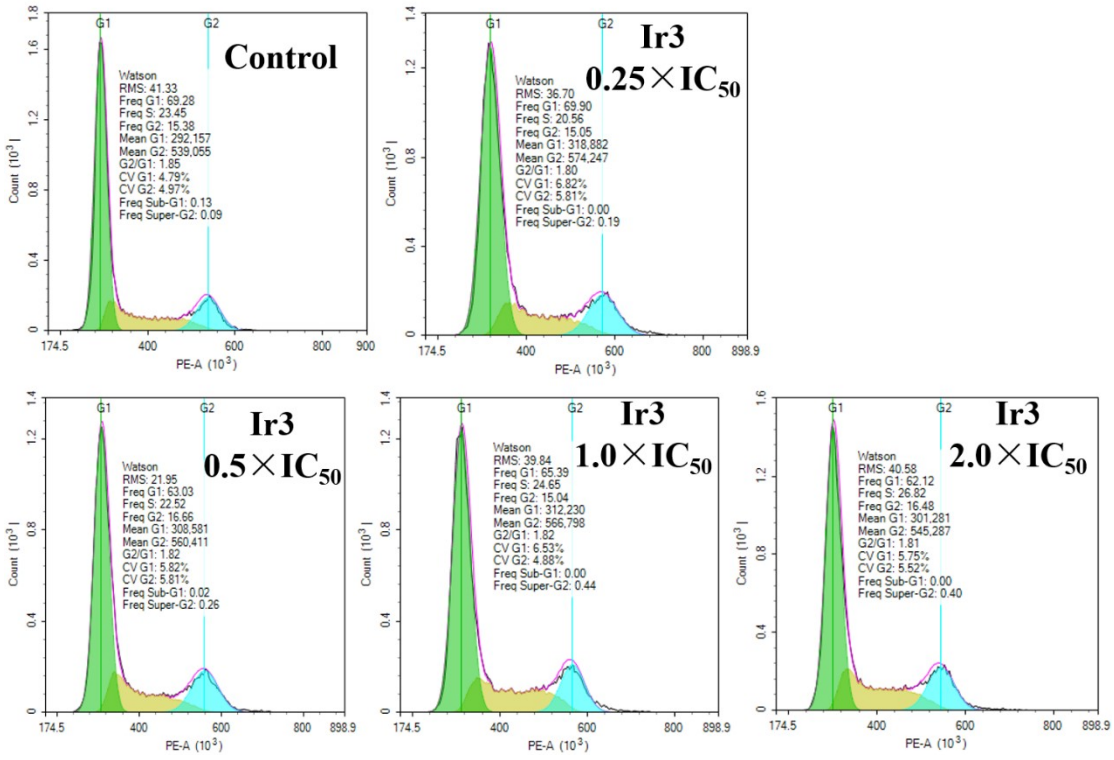


Figure S16 The cell cycle of A549 cells was analyzed by flow cytometry after induced by **Ir3** (concentrations = 0.25, 0.5, 1.0 and 2.0×IC_{50}) for 24 h at 310 K.

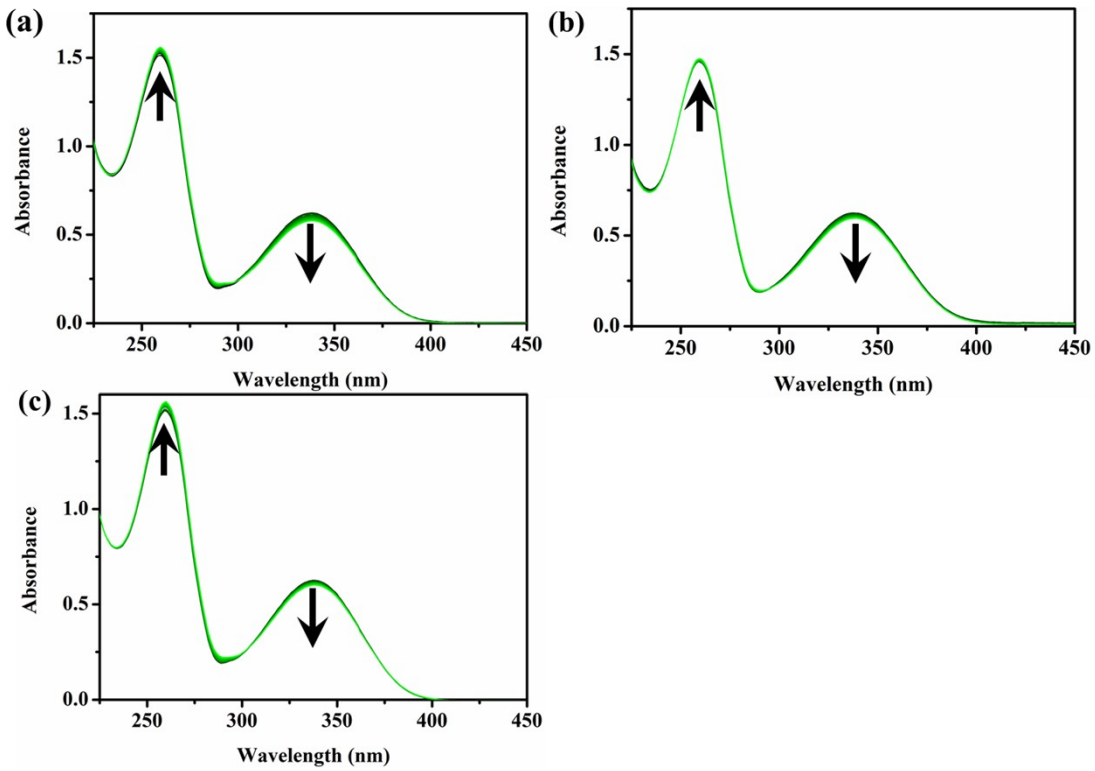


Figure S17 UV-vis spectra of the reaction of NADH (100.0 μM) with **Ir1** (a), **Ir2** (b) and **Ir4** (c) (1.0 μM) in 20% MeOH/80% H_2O (*v*/*v*) at 298 K for 8 h. The arrows show the intensity changes with the increase of complexes.

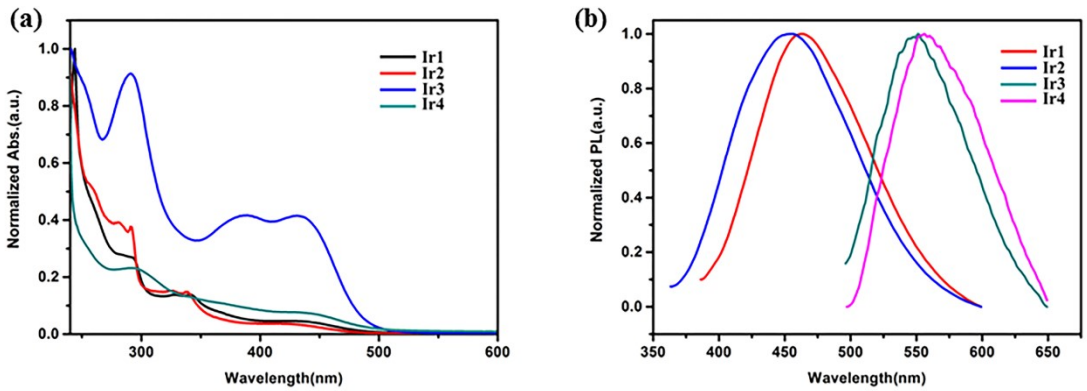


Figure S18 Normalized UV-vis absorption (a) and PL spectra (b) of **Ir1-Ir4**. (DMSO solution, 2.0×10^{-5} mol L^{-1}).

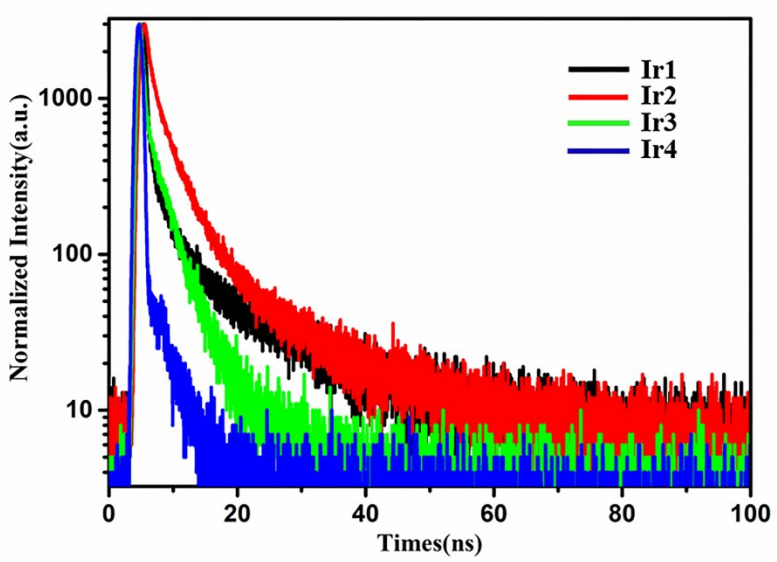


Figure S19 Normalized fluorescence lifetime of **Ir1-Ir4**.

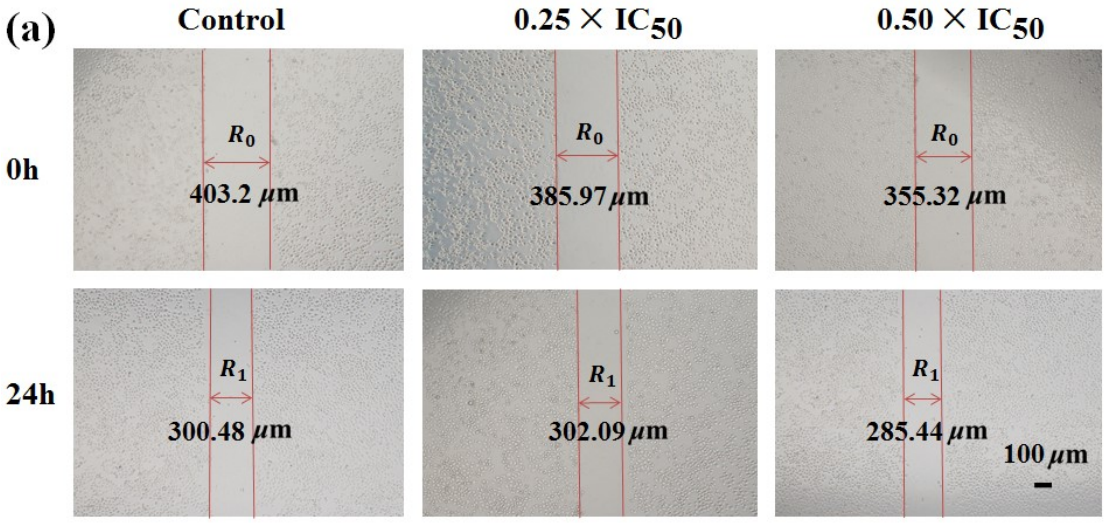


Figure S20 Wound healing assay of A549 cells treated with complex **Ir1** for 24 h (concentrations: 0.25×IC_{50}, 0.50×IC_{50}). (a) Typical images were taken at 0 h and 24 h. The widths of wounds are indicated with the lines (μm). Scale bar: 100 μm.

3 Tables

Table S1 Crystallographic data for **Ir1**.

formula	$C_{35}H_{32}ClIrN_2O{\cdot}0.5C_6H_{14}$
MW	767.36
cryst size (mm)	0.49×0.21×0.17
λ(Å)	0.71073
temp (K)	298
cryst syst	Monoclinic
space group	P2(1)/n
a (Å)	16.4918(14)
b (Å)	10.0684(8)
c (Å)	21.1210(17)
α (°)	90
β (°)	109.031(2)
γ (°)	90
vol ($Å^3$)	3315.4(5)
Z	4
density (calc) ($mg{\cdot}m^{-3}$)	1.537
abs coeff (mm^{-1})	4.140
F(000)	1532
θ range (deg)	2.41 to 25.02
index ranges	$-19 \le h \le 19$, $-11 \le k \le 11$, $-14 \le l \le 25$
reflns collected	15818
indep reflns	5814 [R(int) = 0.0811]
data / restraints / params	5814 / 0 / 394
final R indices [I > 2σ(I)]	R1 = 0.0341, wR2 = 0.0608
GOF	0.960
largest diff peak and hole	1.112 and -0.939

Table S2 Selected bond lengths (Å) and angles (°) for **Ir1.**

Ir–C (Cp*)	2.129(6)
	2.136(6)
	2.158(6)
	2.159(5)
	2.166(5)
Ir–Cp* (centroid)	1.7757
Ir-N	2.098(4)
Ir-O	2.078(4)
Ir-Cl	2.4252(15)
O-Ir-N	87.20(15)
O-Ir-Cl	85.94(12)
N-Ir-Cl	89.93(11)

Table S3 Flow cytometry analysis to determine the percentages of apoptotic cells, using Annexin V-FITC vs PI staining, after exposing A549 cells to **Ir3**.

	Population (%)				
	Ir concentration	**Viable**	**Early apoptosis**	**Late apoptosis**	**Non-viable**
Ir3	0.5 × IC_{50}	87.04±1.2	2.09±0.1	10.73±0.6	0.14±0.09
	1.0 × IC_{50}	82.76±1.2	1.70±0.1	15.16±0.6	0.38±0.09
	2.0 × IC_{50}	81.02±1.6	2.34±0.4	16.32±1.2	0.32±0.90
	3.0 × IC_{50}	68.07±0.9	3.19±0.2	26.48±1	2.26±0.70
Control		92.79±1.5	3.17±0.2	3.90±0.9	0.14±0.05

Table S4 The mitochondrial membrane polarization of A549 cells induced by **Ir3**.

	Population (%)		
	Ir Concentration	**JC-1 Aggregates**	**JC-1 Monomers**
Ir3	0.25 × IC_{50}	75.90±0.8	24.10±0.3
	0.5 × IC_{50}	74.13±0.8	25.87±0.7
	1.0 × IC_{50}	73.65±2.3	26.35±0.5
	2.0 × IC_{50}	72.51±1.2	27.49±4.3
Negative Control		92.09±2.8	7.91±0.9
Positive Control		25.15±1.6	74.85±3.9

Table S5 UV-vis absorption and PL spectra peak position, absolute fluorescence quantum yield (AFQY), fluorescence lifetime for **Ir1-Ir4**.

	Abs. (nm)	**PL (nm)**	**AFQY (%)**	**lifetime (*μ*s)**
Ir1	298，340	463	0.02%	1.198
Ir2	282，345	454	0.73%	0.725
Ir3	295，390，436	548	0.83%	0.388
Ir4	300，440	556	0.93%	0.127