Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting Information

Aggregation-Induced Phosphorescent Emission-Active Ir(Ⅲ) Complexes with Long Lifetime for Specific Mitochondrial Imaging and Tracking

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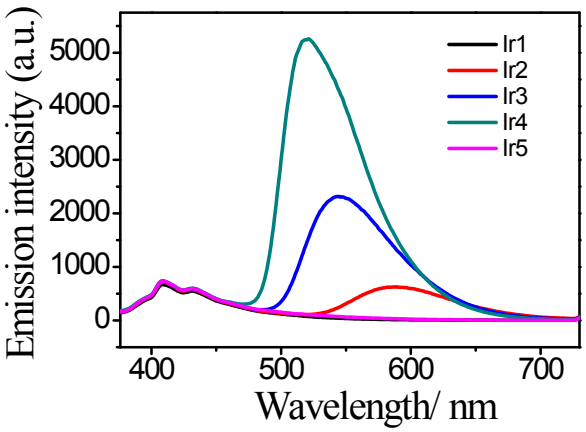

Fig.S1 Emission spectra of **Ir1-Ir5** in CH_2Cl_2 at room temperature. ($c=1\times10^{-5}M$)

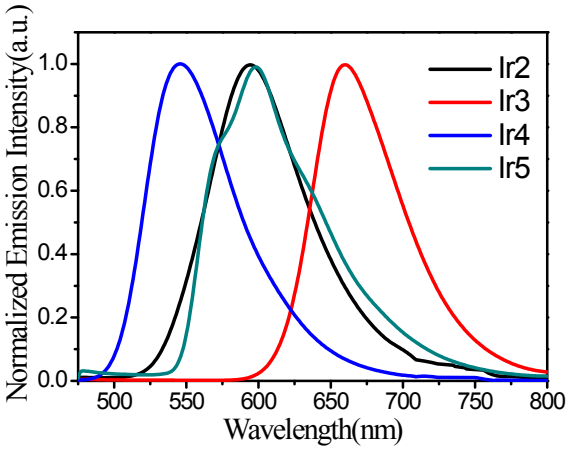

Fig. S2 The normalized emission spectra of **Ir2-Ir4** in solid state

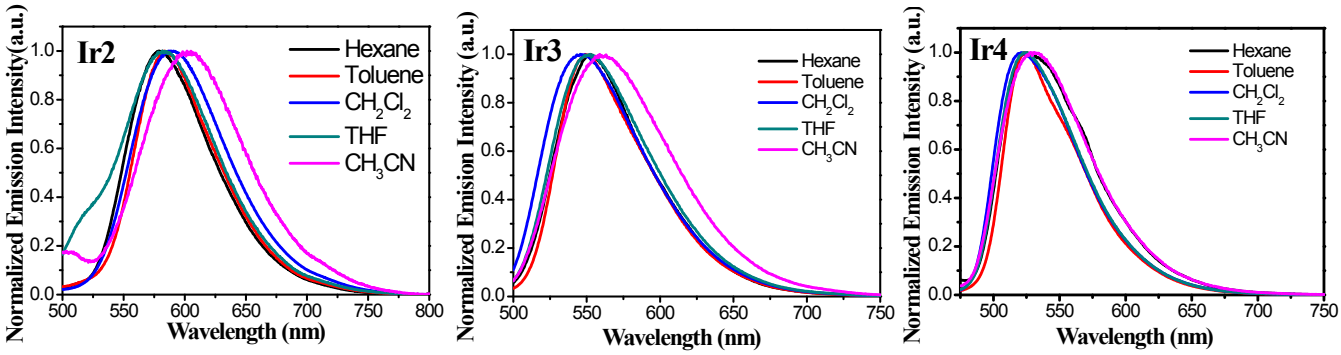

Fig. S3 Normalized emission spectra of **Ir2, Ir3**, **Ir4** in different solvents

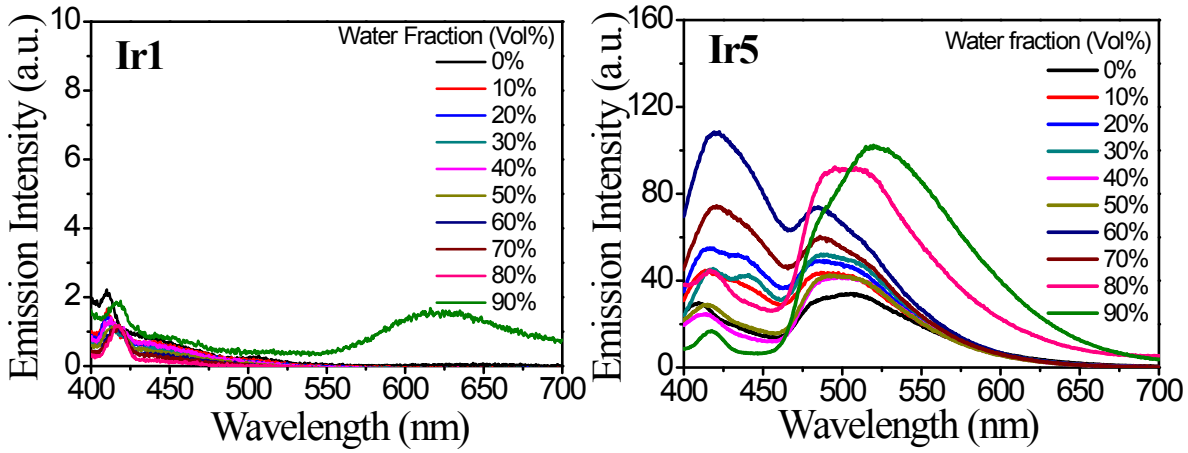

Fig. S4 Emission spectra of complexes **Ir5** (c = 1.0×10^{-5} M) in CH_3CN–water mixtures with different water fractions (0–90%).

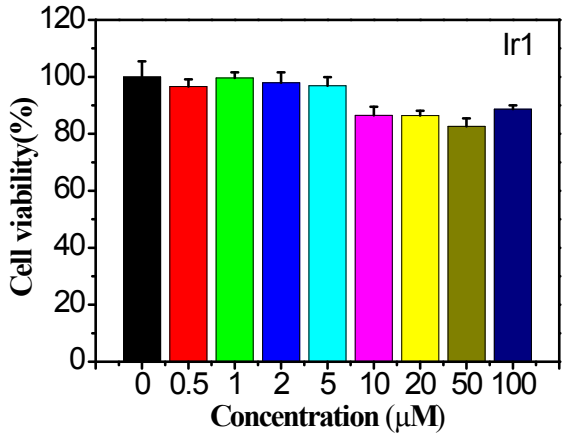

Fig. S5 Cytotoxicity assay for **Ir1** in HeLa cells, after 12 h of incubation

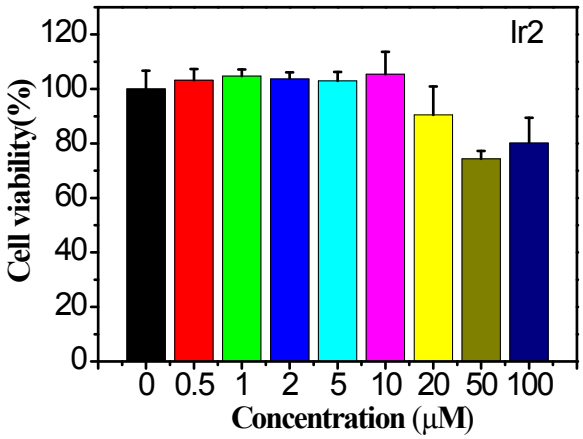

Fig. S6 Cytotoxicity assay for **Ir2** in HeLa cells, after 12 h of incubation

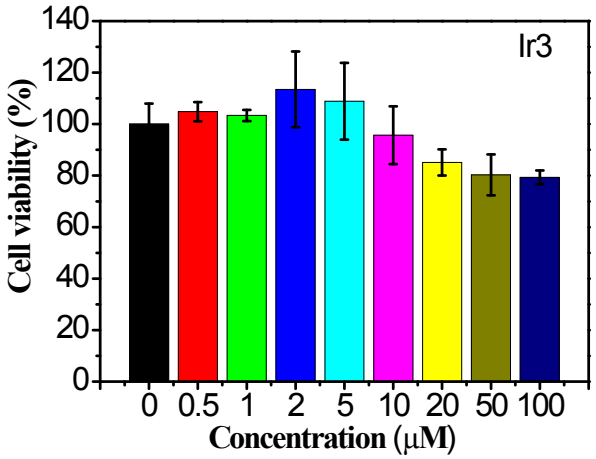

Fig. S7 Cytotoxicity assay for **Ir3** in HeLa cells, after 12 h of incubation

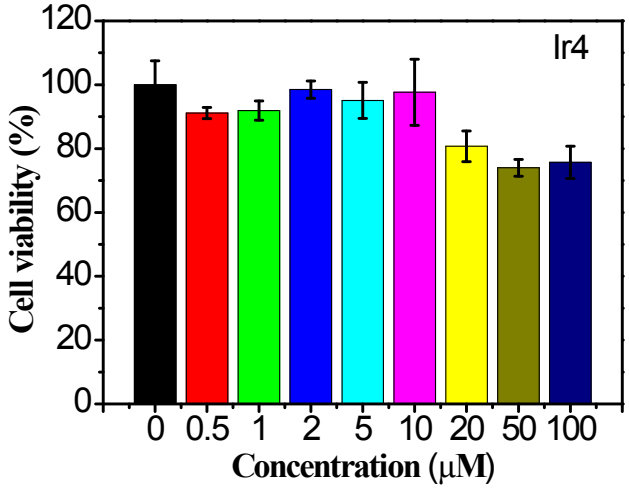

Fig. S8 Cytotoxicity assay for **Ir4** in HeLa cells, after 12 h of incubation

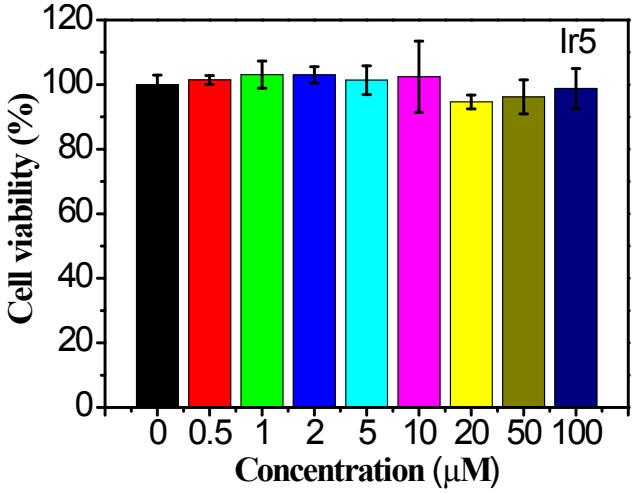

Fig. S9 Cytotoxicity assay for **Ir5** in HeLa cells, after 12 h of incubation

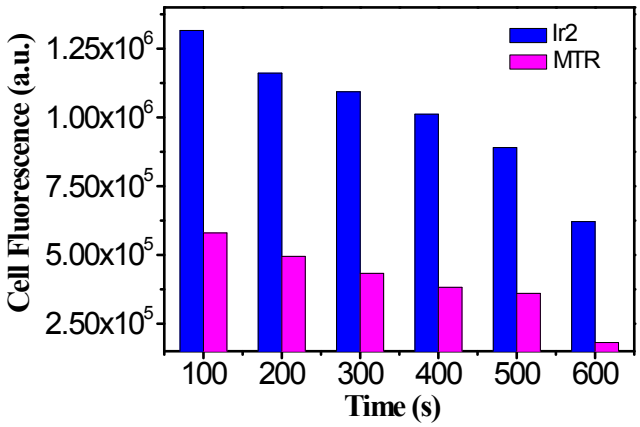

Fig. S10 The anti-bleaching properties of **Ir2** , the fluorescent intensity of **Ir2** (blue) and MTR (purple) with livig HeLa cells with increasing scan time. HeLa cells were treated with 10 μM of **Ir2**, followed by 50 nM of MTR.

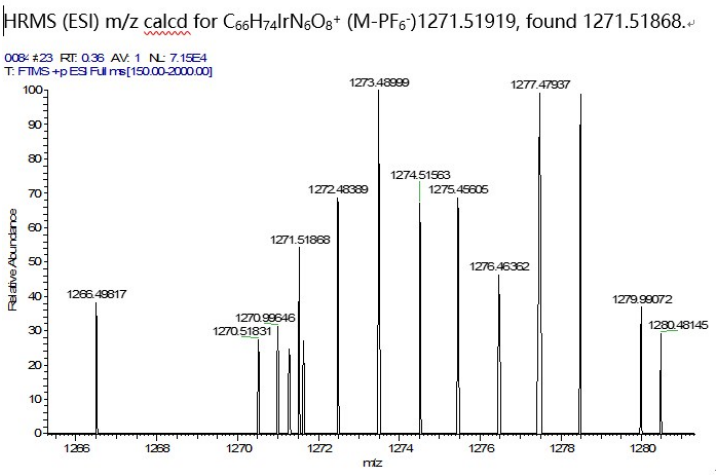

Fig. S11 HRMS spectrum of **Ir1**

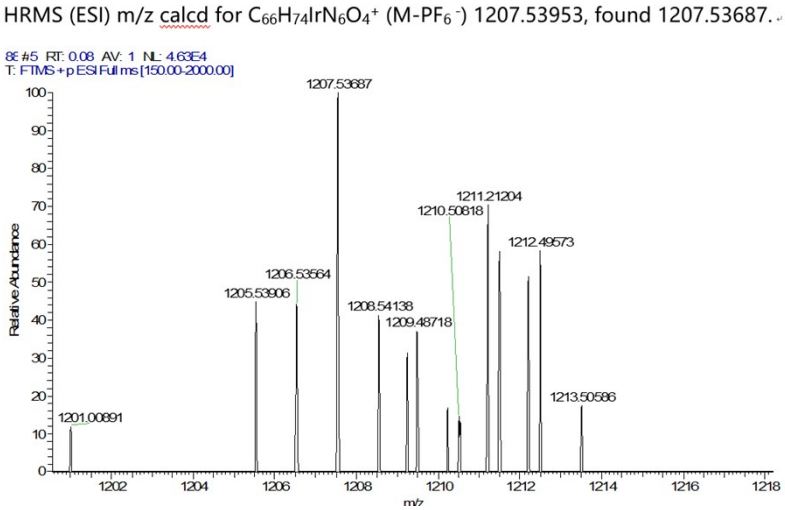

Fig. S12 HRMS spectrum of **Ir2**

HRMS (ESI) m/z calcd for $C_{62}H_{66}IrN_6O_4^+$ ($M-PF_6^-$) 1151.47693, found 1151.47693.

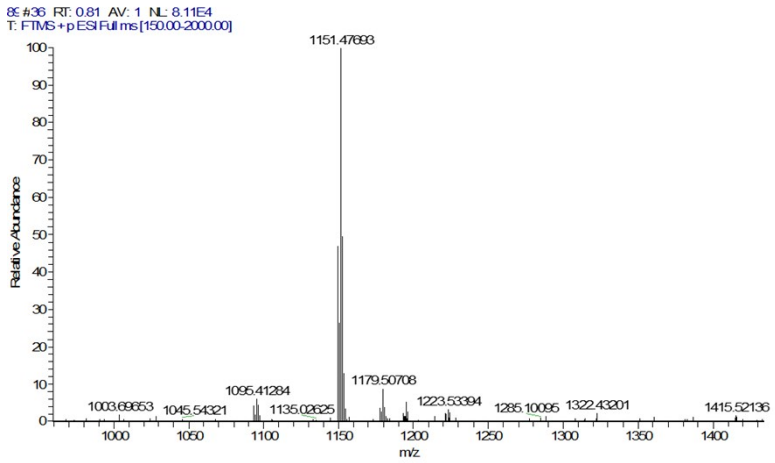

Fig. S13 HRMS spectrum of **Ir3**

HRMS (ESI) m/z calcd for $C_{62}H_{62}F_4IrN_6O_4^+$ ($M-PF_6^-$) 1223.43924, found 1223.43945.

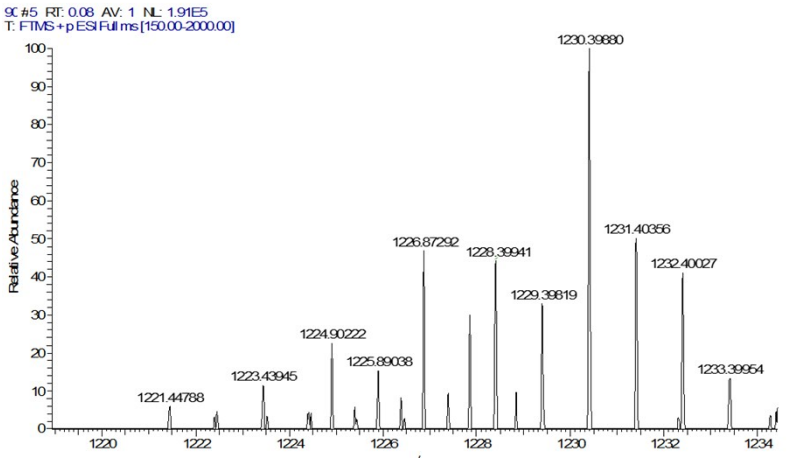

Fig. S14 HRMS spectrum of **Ir4**

HRMS (ESI) m/z calcd for $C_{66}H_{62}F_{12}IrN_6O_4^+$ ($M-PF_6^-$) 1423.42647, found 1423.44092.

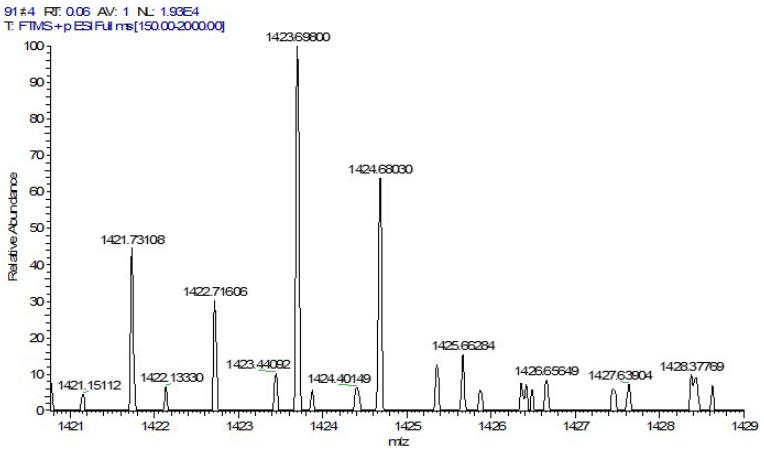

Fig. S15 HRMS spectrum of **Ir5**

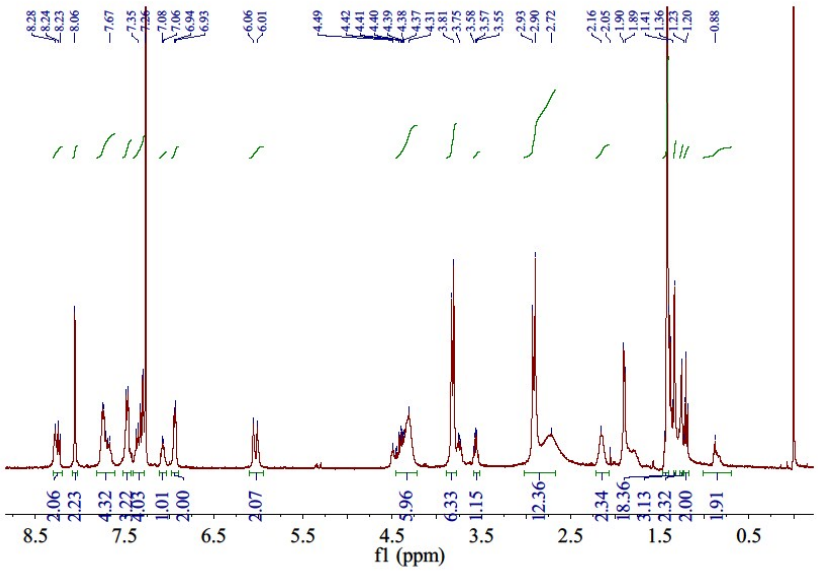

Fig. S16 ^{1}H NMR spectrum of **Ir1**

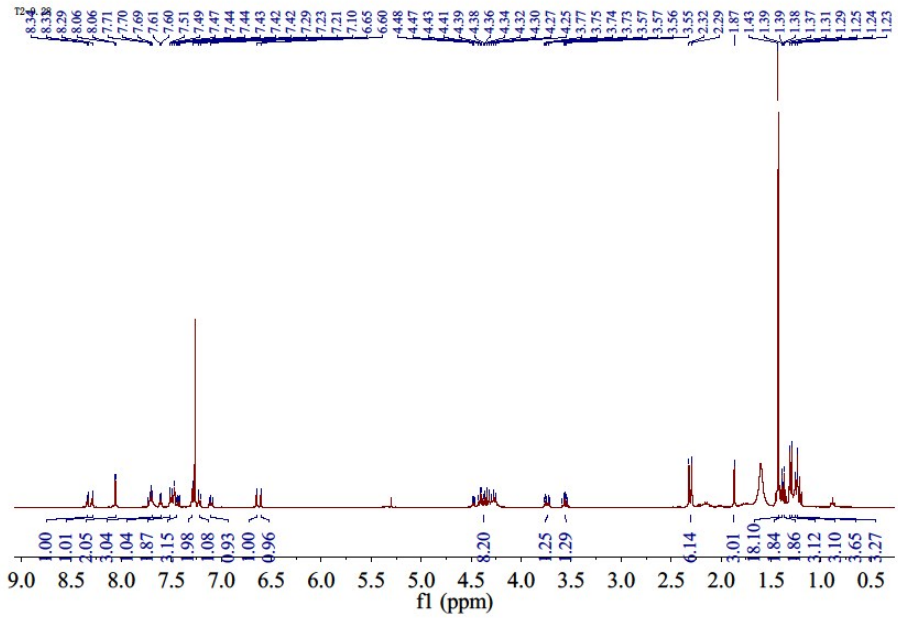

Fig. S17 ^{1}H NMR spectrum of **Ir2**

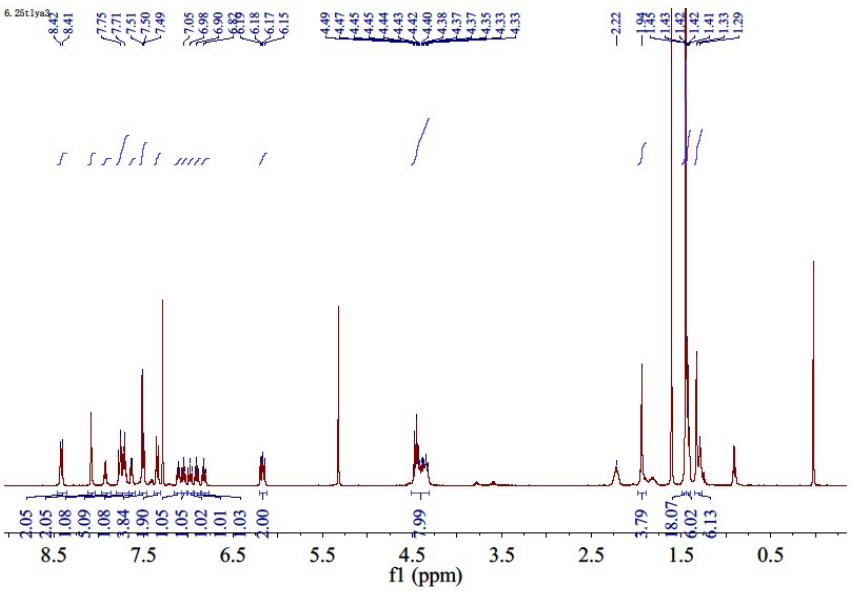

Fig. S18 ^{1}H NMR spectrum of **Ir3**

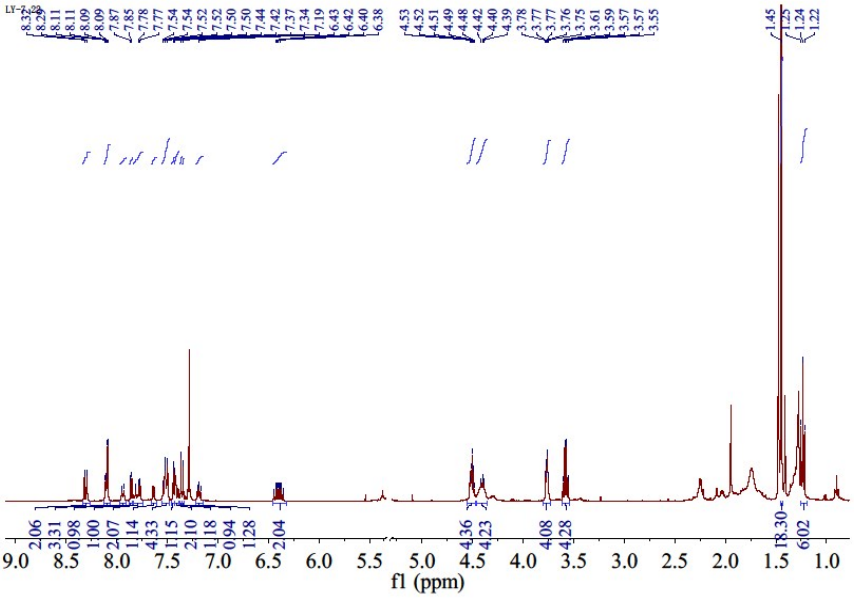

Fig. S19 ^{1}H NMR spectrum of **Ir4**

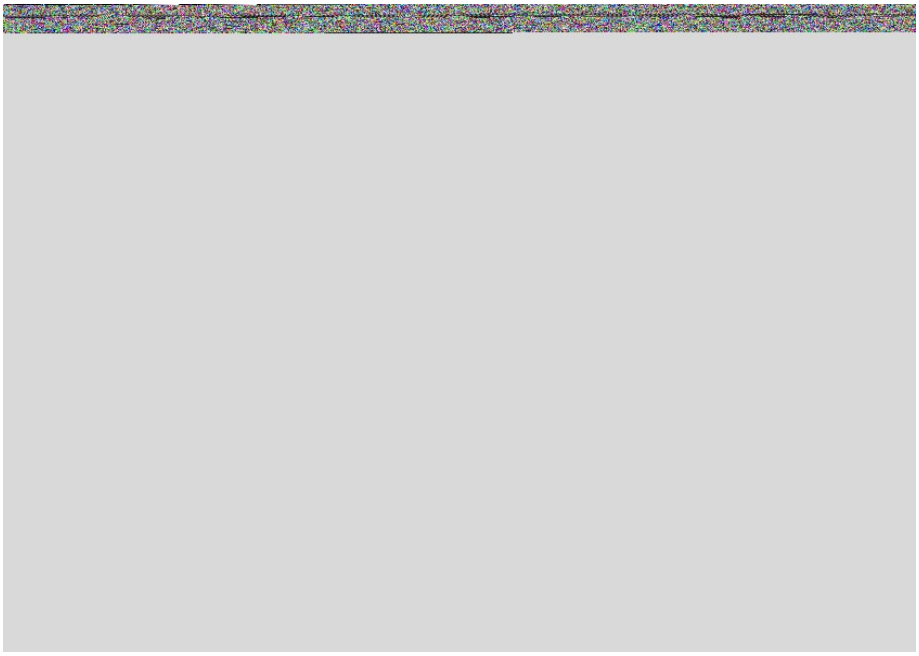

Fig. S20 ^{1}H NMR spectrum of **Ir5**

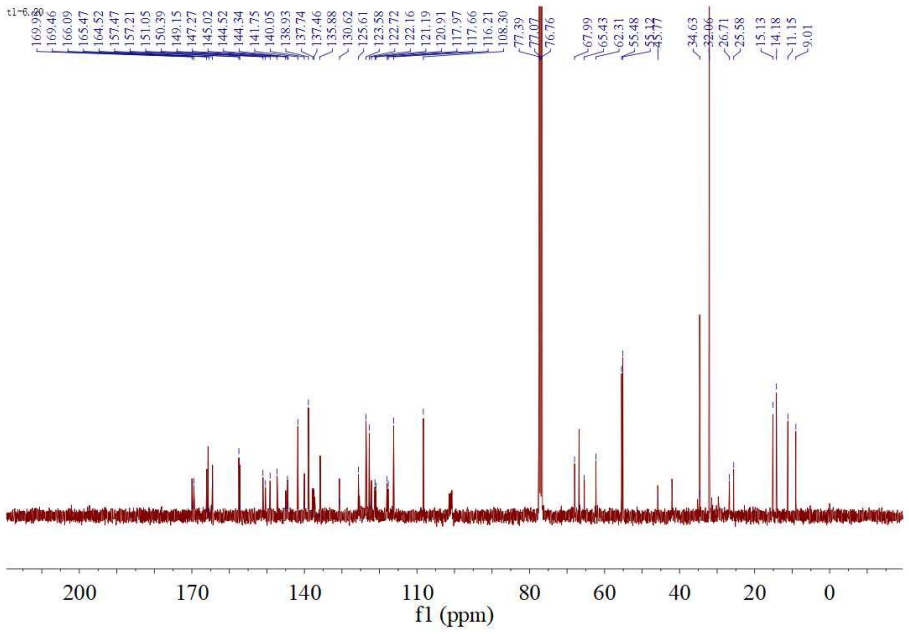

Fig. S21 ^{13}C NMR spectrum of **Ir1**

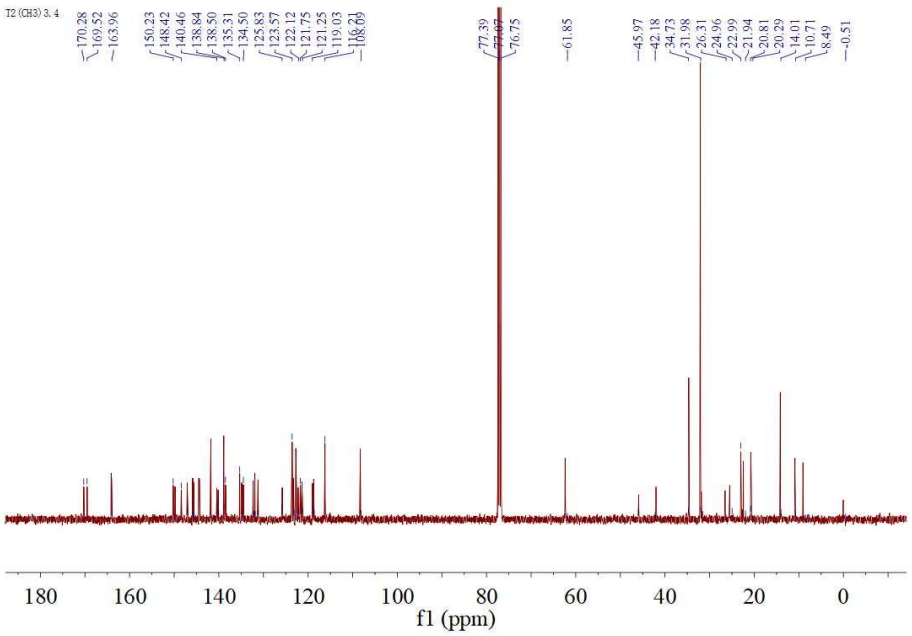

Fig. S22 ^{13}C NMR spectrum of **Ir2**

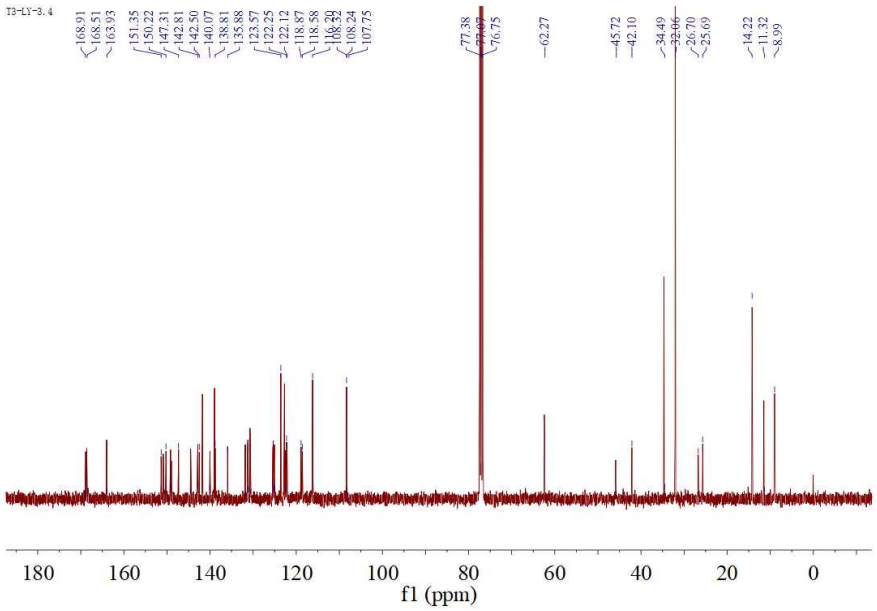

Fig. S23 ^{13}C NMR spectrum of **Ir3**

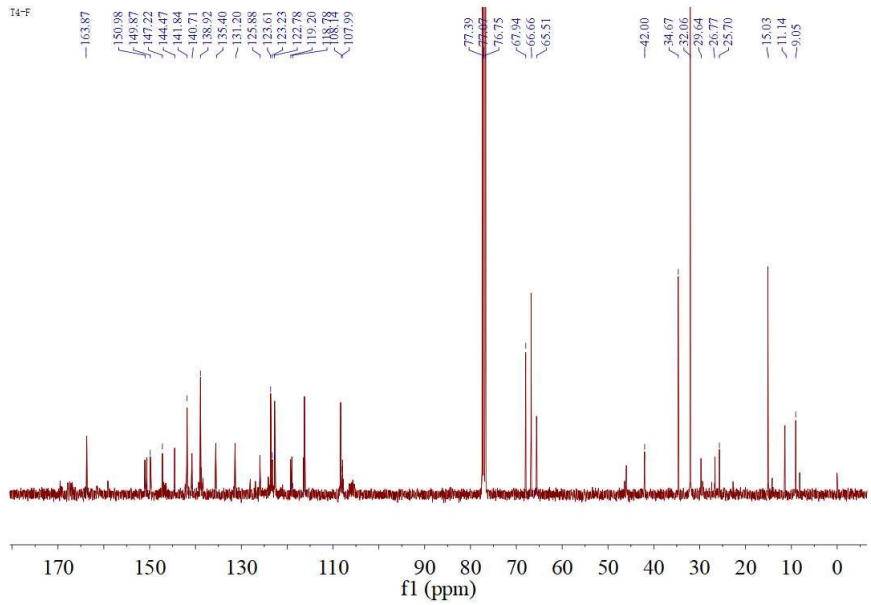

Fig. S24 ^{13}C NMR spectrum of **Ir4**

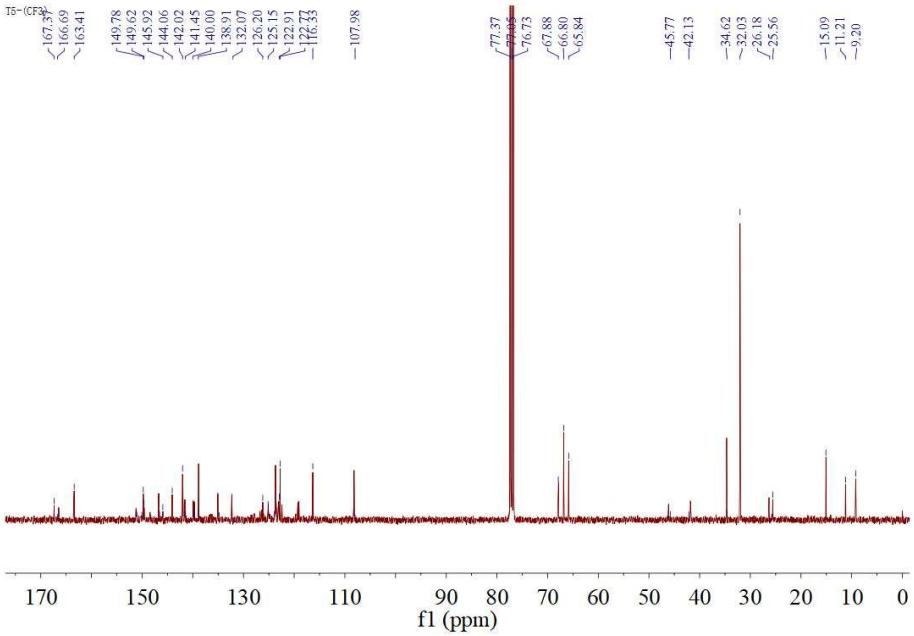

Fig. S24 ^{13}C NMR spectrum of **Ir5**

Table S1 Crystallographic data for complexes **Ir3**

Compound	Ir3
Formula	$C_{62}H_{66}F_6IrN_6O_4P$
Formula weight	1296.37
Crystal system	Monoclinic
Space group	P 21/n
a [Å]	15.9678(7)
b [Å]	16.1793(8)
c [Å]	26.2102(13)

α (°)	90
β (°)	96.948(2)
γ (°)	90
Volume [Å3]	6721.6(6)
T [K]	153 K
Z	4
F(000)	2632
Index ranges	$-18 \le h \le 18, -19 \le k \le 18, -31 \le l \le 21$
μ (Mo-Kα)(mm-1)	1.281
θ, deg	2.28 to 25.21
data/restraints/par ameters	11829/356/731
R_1^a , wR_2^b (I>2σ(I))	0.0465,0.0702
R_1^a , wR_2^b	0.1221,0.1343
GOF	1.080

Table S2 Selected bond lengths (Å) and angles (°) for **Ir3**

Ir-N3	2.13	N5-Ir-C59	80.70	N3-Ir-N5	91.36
Ir-N4	2.04	N3-Ir-N6	75.20	N3-Ir-C59	100.58
Ir-N5	2.05	C48-Ir-C59	88.38	N3-Ir-C48	170.08
Ir-N6	2.16	N6-Ir-C48	96.06	N6-Ir-C59	174.79
Ir-C59	2.01	N5-Ir-N6	96.21		
Ir-C48	2.01	N4-Ir-N5	172.30		
N4-Ir-C48	80.66	N4-Ir-N3	94.48		