Supporting Information

Heteronuclear phosphorescent iridium(III) complexes with tunable photophysical and excited-state properties by chelating BF_2 moiety for application in bioimaging

Huibin Sun,[‡a] Lijuan Yang,[‡ac] Huiran Yang,[a] Shujuan Liu,[a] Wenjuan Xu,[a] Xiangmei Liu,[a] Zhenzhen Tu,[a] Haiquan Su,[b] Qiang Zhao,*[a] and Wei Huang*[ab]

[a] *Key Laboratory for Organic Electronics & Information Displays (KLOEID) and Institute of Advanced Materials (IAM), Nanjing University of Posts & Telecommunications (NUPT), 9 Wenyuan Road, Nanjing 210046, P. R. China. Fax: +86 25 8586 6396, Tel: +86 25 8586 6396; wei-huang@njupt.edu.cn; iamqzhao@njupt.edu.cn*

[b] *Jiangsu-Singapore Joint Research Center for Organic/Bio-Electronics and Institute of Advanced Materials, Nanjing University of Technology, Nanjing 211816, China. Fax: +86 25 5813 9988; Tel: +86 25 5813 9001.*

[c] *School of Chemistry and Chemical Engineering, Inner Mongolia University, Hohhot, Inner Mongolia 010021, P. R. China.*

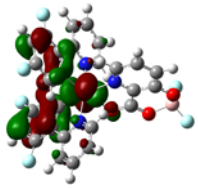
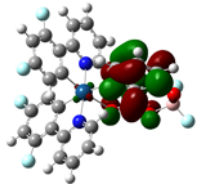
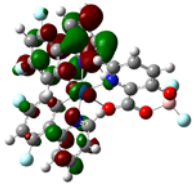
Table S1 Crystal data and refinement parameters for complex **2b**

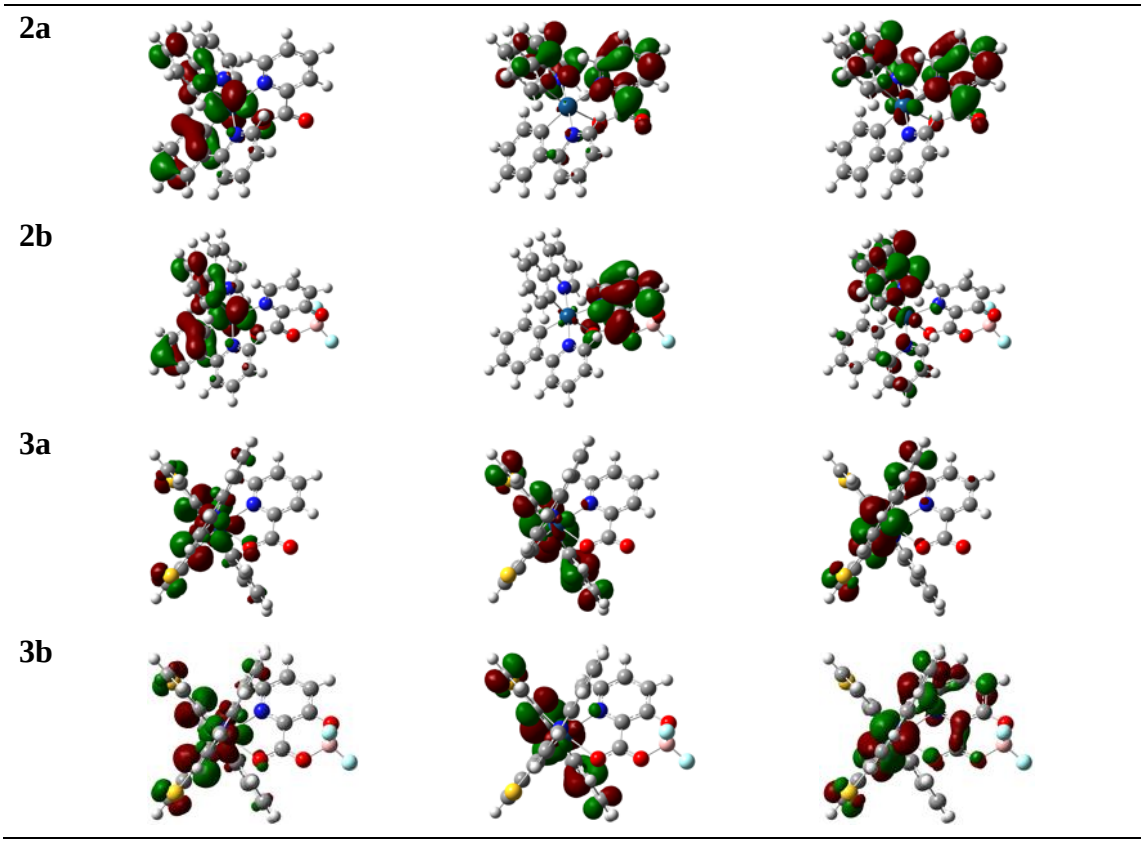
empirical formula	$[IrC_{28}H_{19}N_3F_2BO_3](CH_2Cl_2)$
formula weight	771.42
crystal system	orthorhombic crystal system
space group	$Pna2_1$
a (Å)	12.522(3)
b (Å)	22.397(5)
c (Å)	9.999(2)
V ($Å^3$)	V ($Å^3$)
Z	4
D(calcd) (g cm^{-3})	1.827
μ (mm^{-1})	5.002
F(000)	1496
scan type	ω-2θ
R_1, wR_2	0.0266, 0.0681
goodness of fit	1.047

Table S2. The selected bond length of calculation results of **2b** compared with the X-Ray crystallography results

Selected bond	X-Ray crystallography results	Caluclated bond lengths
Ir1-C11	1.994(5)	2.01719
Ir1-C12	1.991(5)	2.00388
Ir1-N1	2.059(4)	2.06565
Ir1-N2	2.036(4)	2.07907
Ir1-N3	2.150(5)	2.22634
Ir1-O1	2.242(3)	2.24965
B1-O2	1.510(10)	1.53785
B1-O3	1.385(10)	1.50508
B1-F1	1.383(12)	1.37448
B1-F2	1.323(11)	1.35901

Table S3. HOMOs and LUMOs distributions of **1a-3a** and **1b-3b** at the lowest singlet state

	HOMO	LUMO	LUMO+1
1a			
1b			



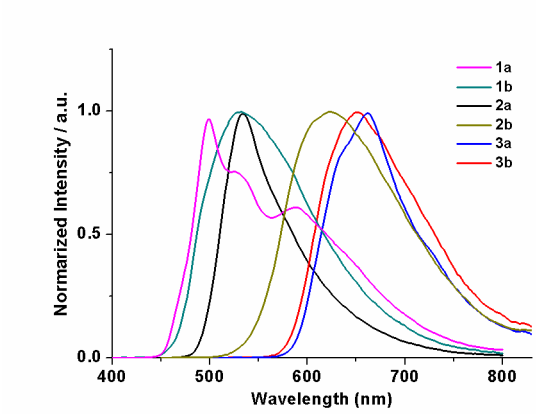


Fig. S1. Emission spectra (excited at 365 nm) in solid state.

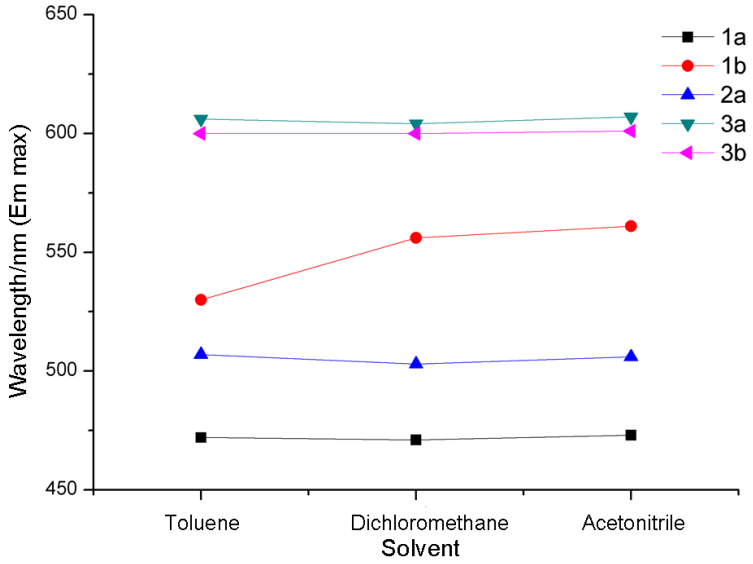


Fig. S2. The maximum emission peak changes of the complexes with different solvent.

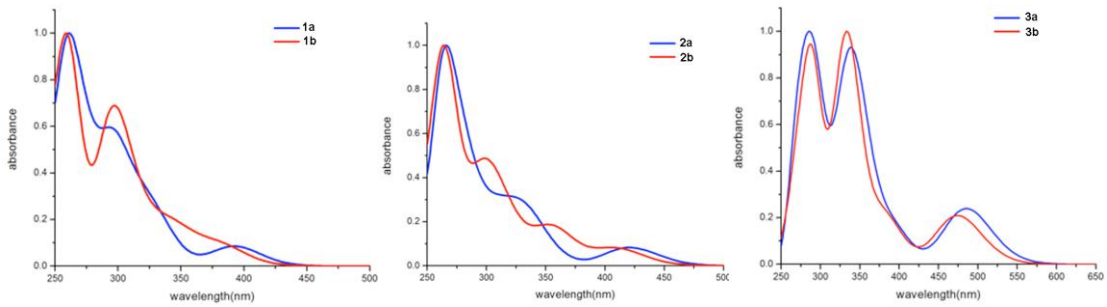


Fig. S3. The calculated absorption spectra of **1a**-**3a** and **1b**-**3b** in CH_2Cl_2 solution.

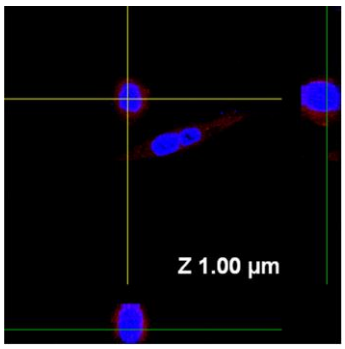


Fig. S4 overlap Z-scan confocal image of living HeLa cells incubated with **3a** and DAPI.