

ELECTRONIC SUPPLEMENTARY INFORMATION

Novel Ruthenium(II) and Iridium(III) BODIPY Dyes: insights into their application in vitro Photodynamic Therapy

Nuray Esra Aksakal, Esra Tanriverdi Eçik*, Hasan Hüseyin Kazan, Gönül Yenilmez Çiftçi,

Fatma Yuksel*

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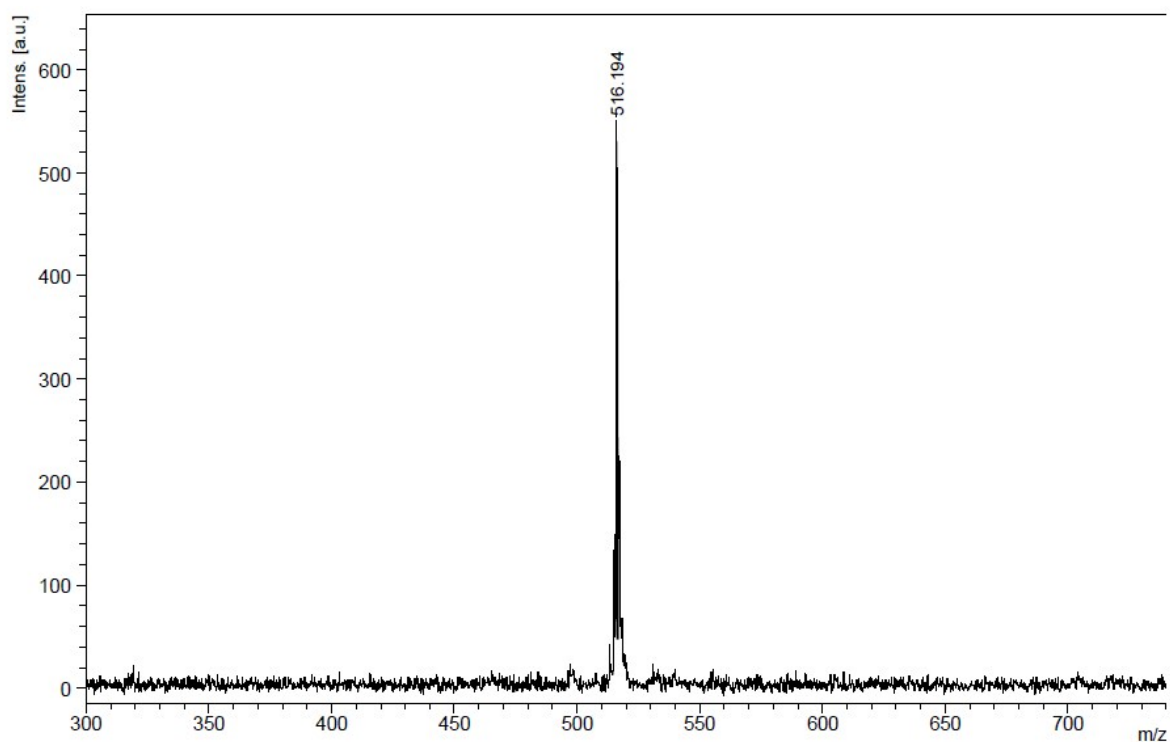


Fig. S1 MALDI-TOF spectrum of BD.

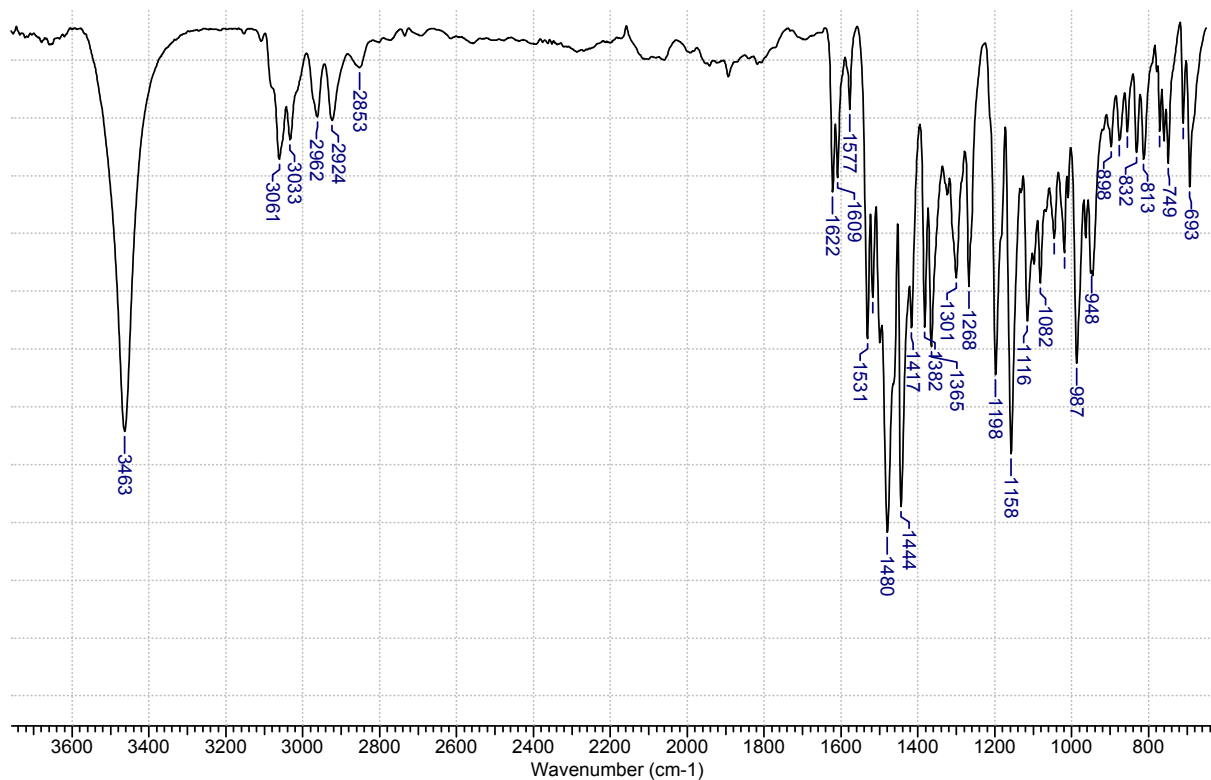


Fig. S2 FT-IR Spectrum of BD.

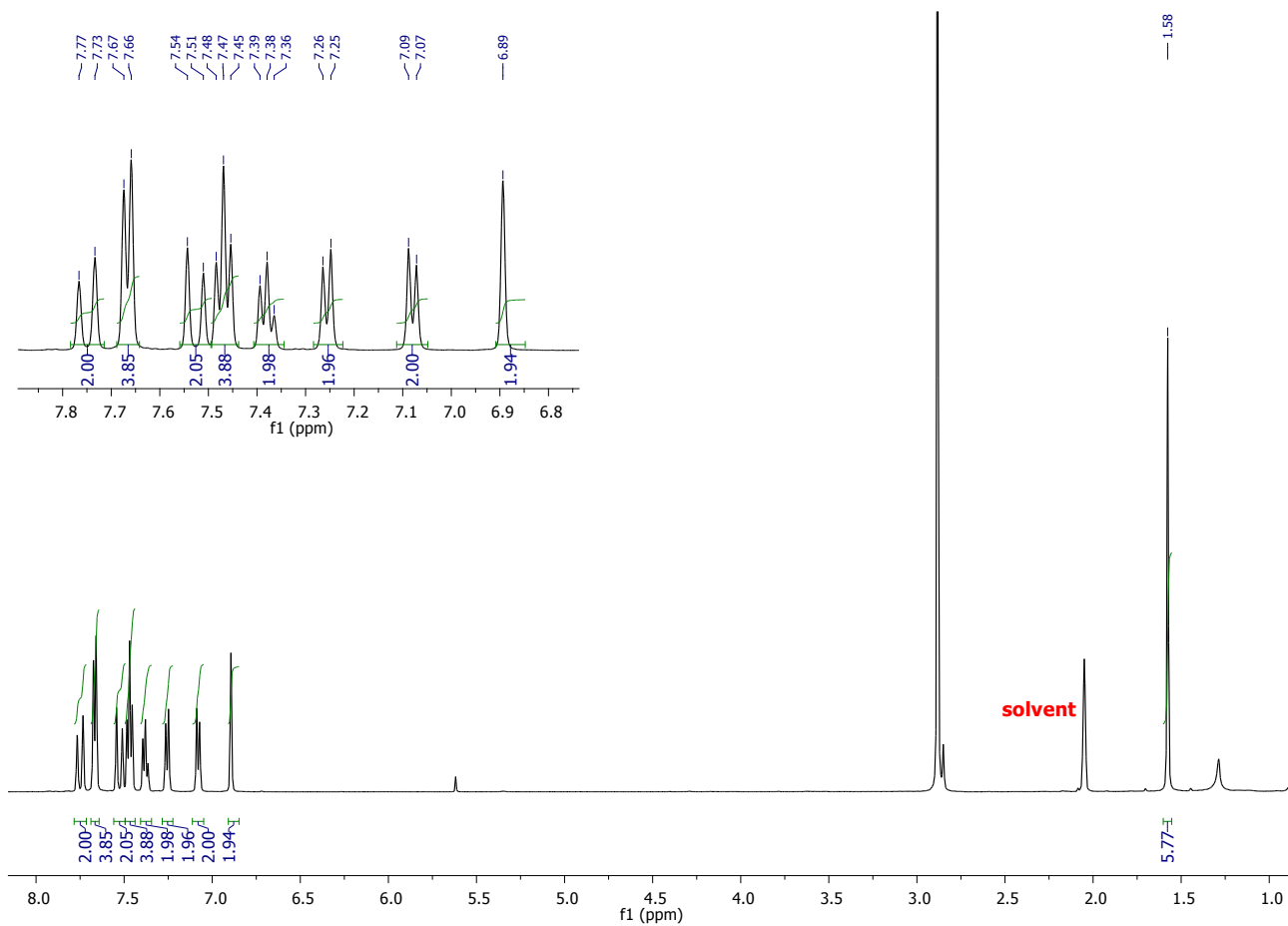


Fig. S3 $^1\text{H-NMR}$ spectrum of BD.

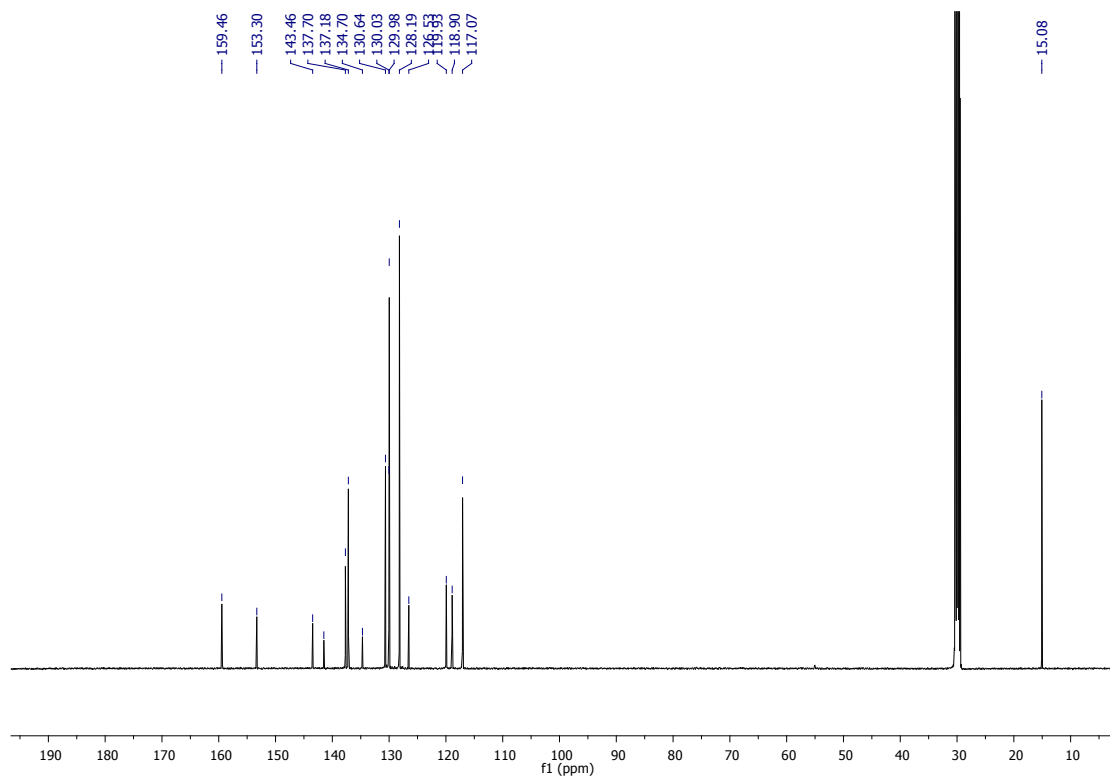


Fig. S4 ^{13}C -NMR spectrum of **BD**.

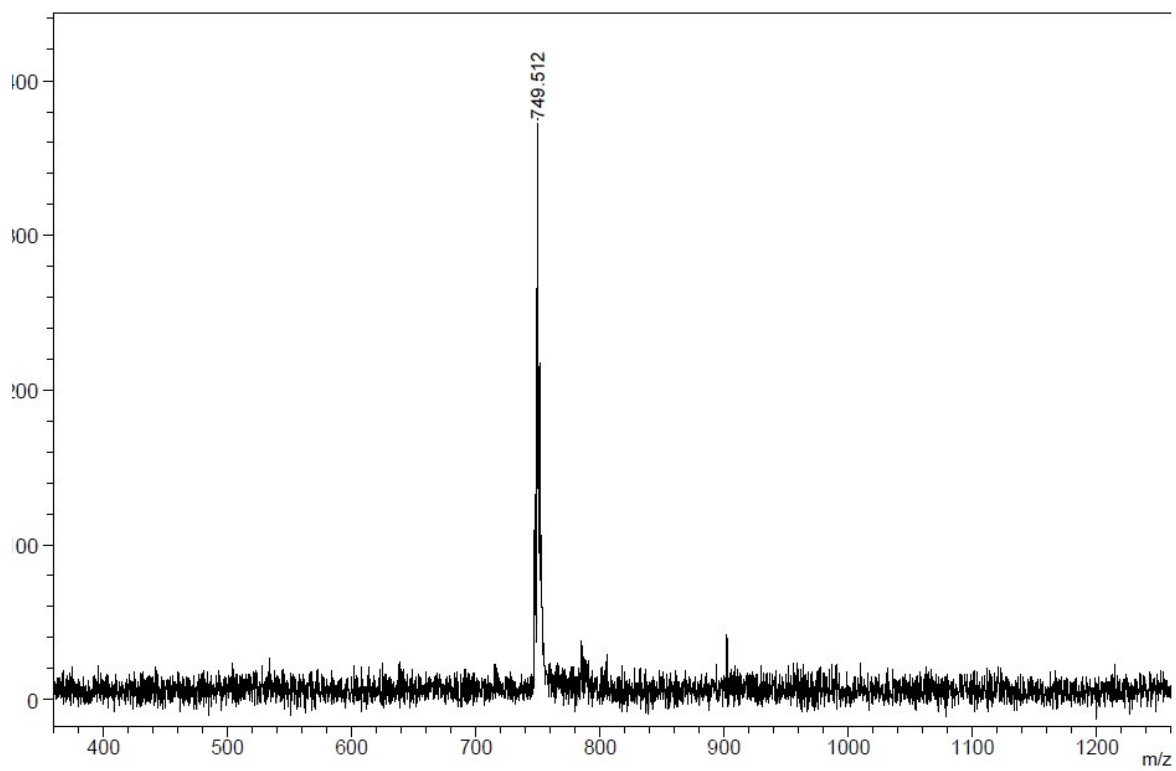


Fig. S5 MALDI-TOF spectrum of **4**.

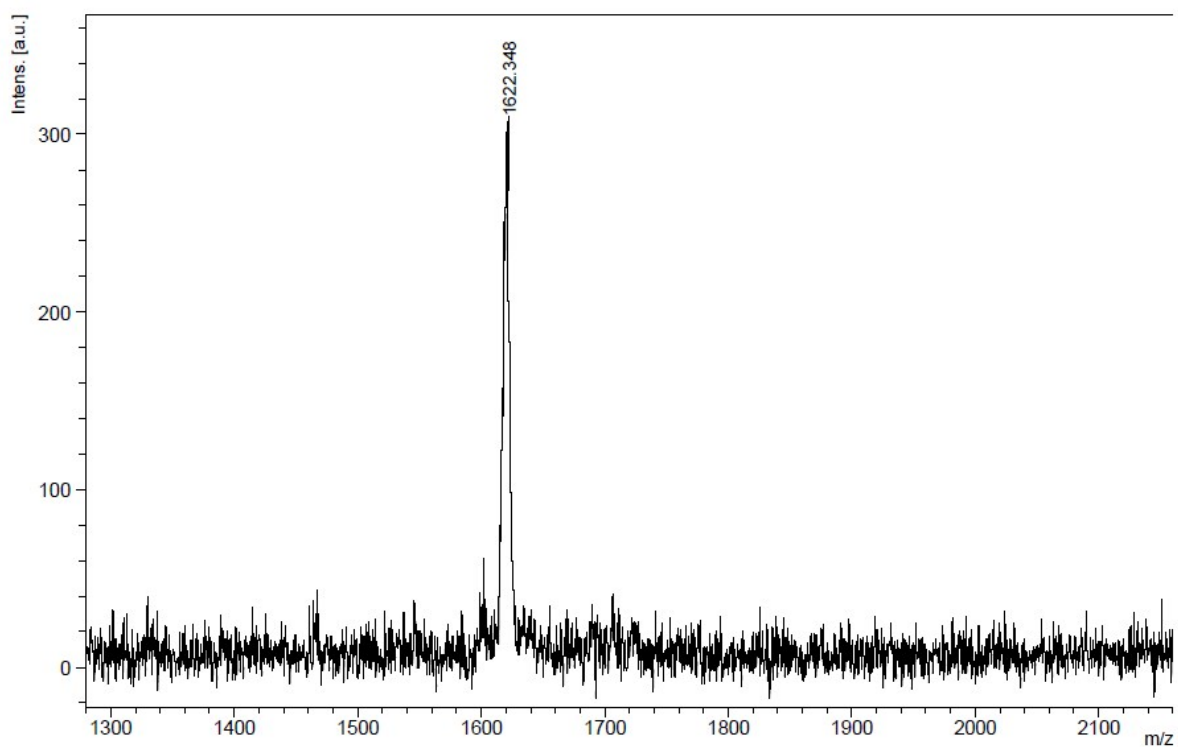


Fig. S6 MALDI-TOF spectrum of Ru- BD.

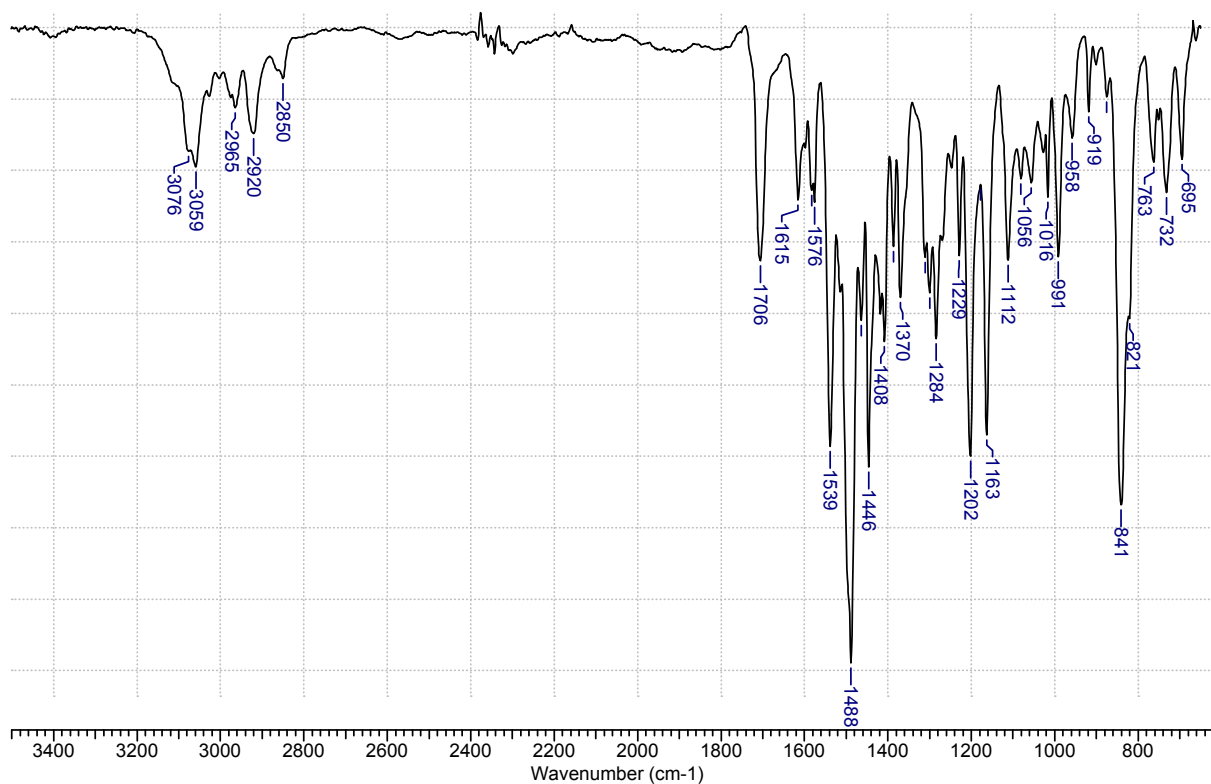


Fig. S7 FT-IR Spectrum of Ru- BD.

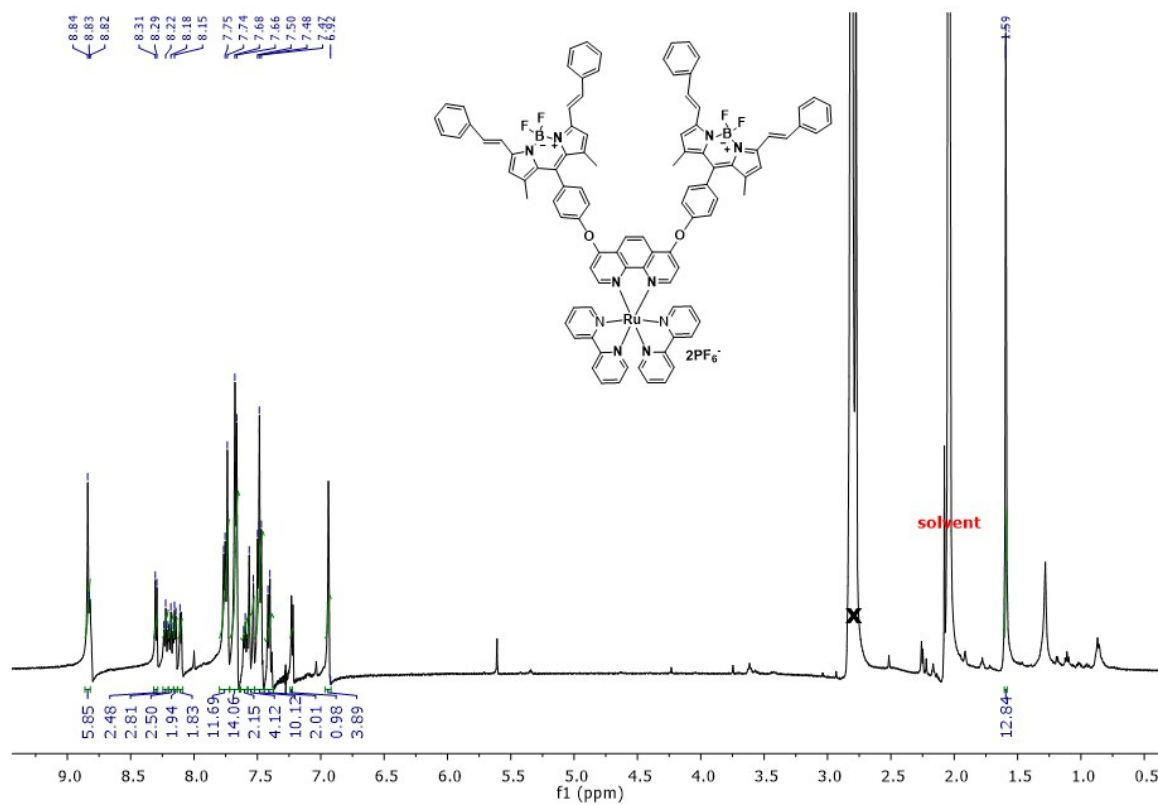


Fig. S8 ¹H-NMR spectrum of Ru-BD.

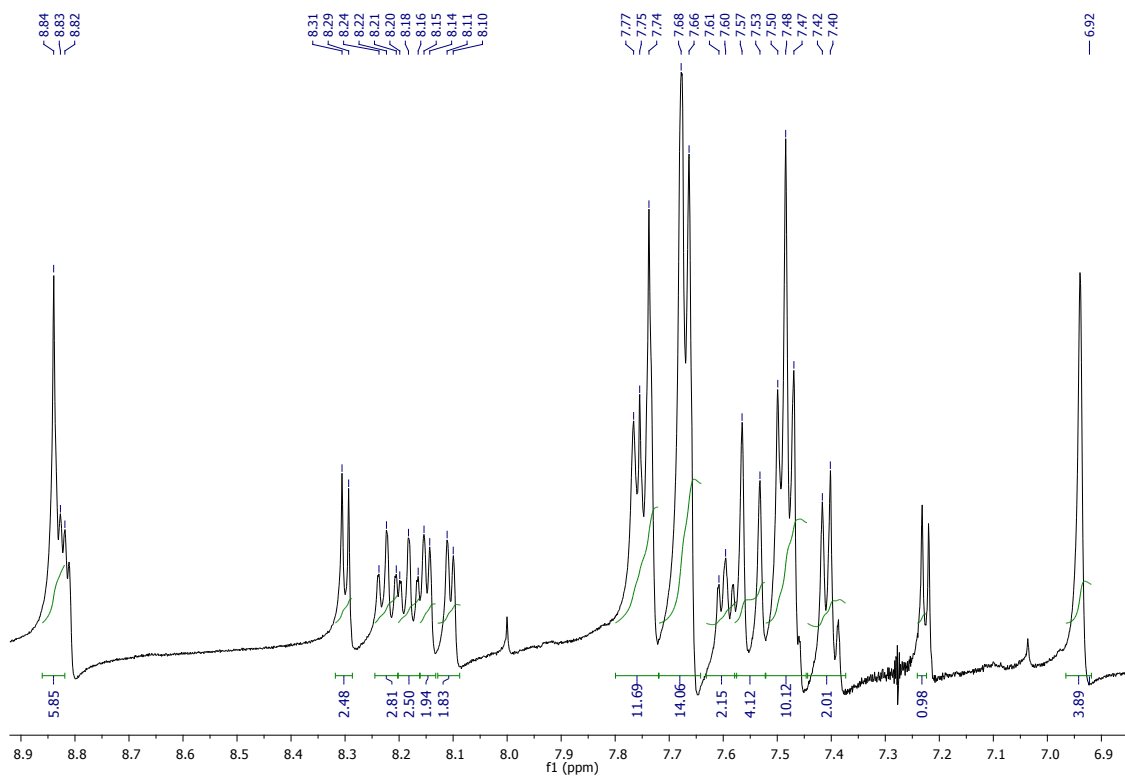


Fig. S9 Aromatic region of ¹H-NMR spectrum of Ru-BD.

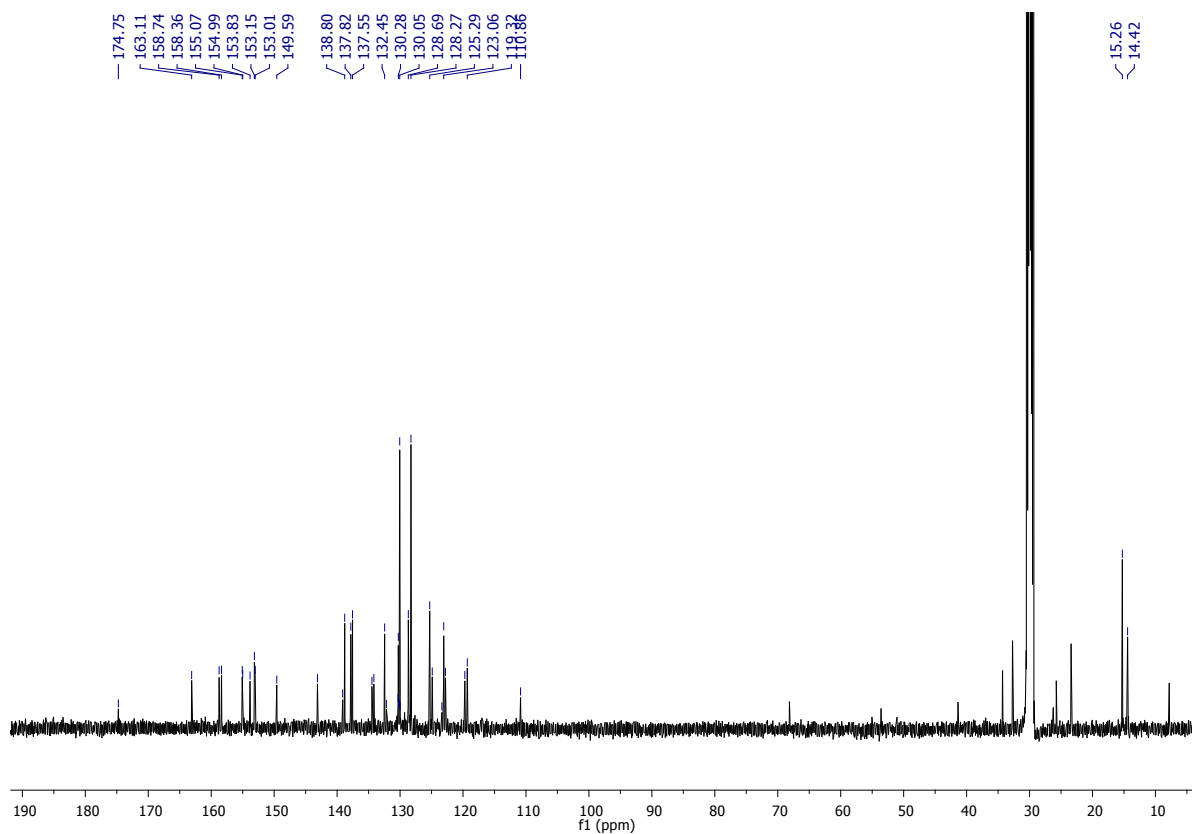


Fig. S10 ^{13}C -NMR spectrum of Ru-BD.

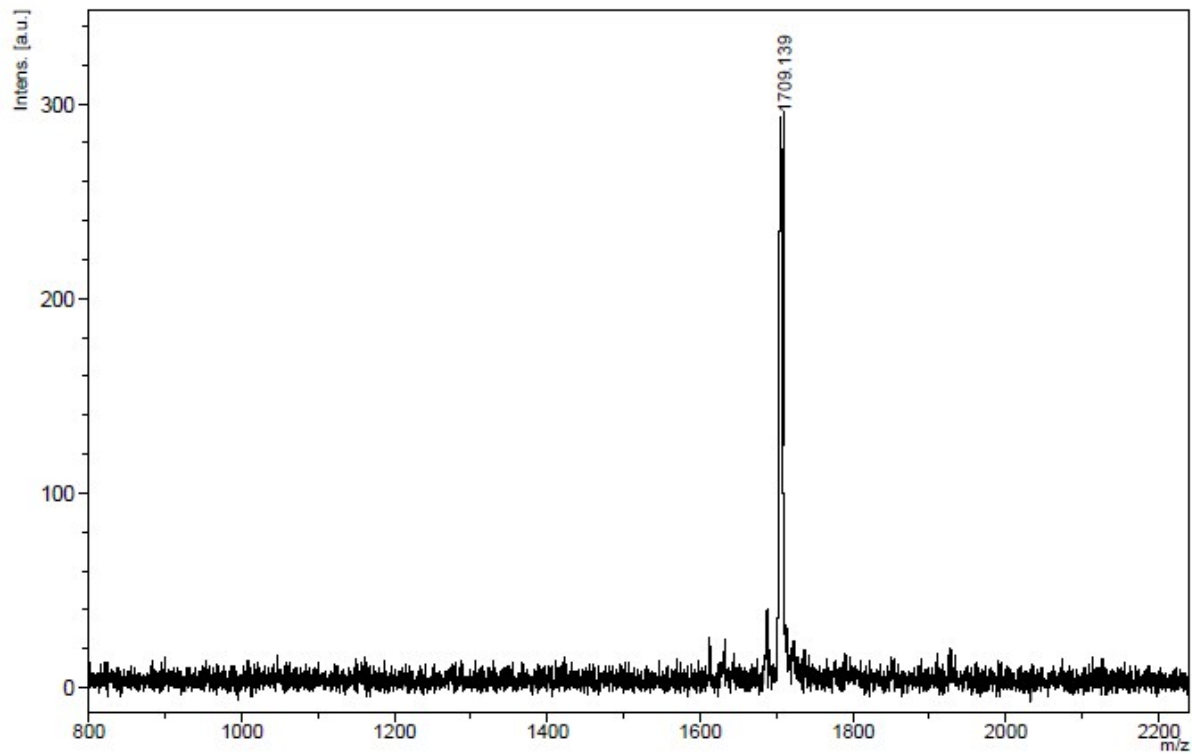


Fig. S11 MALDI-TOF spectrum of Ir-BD.

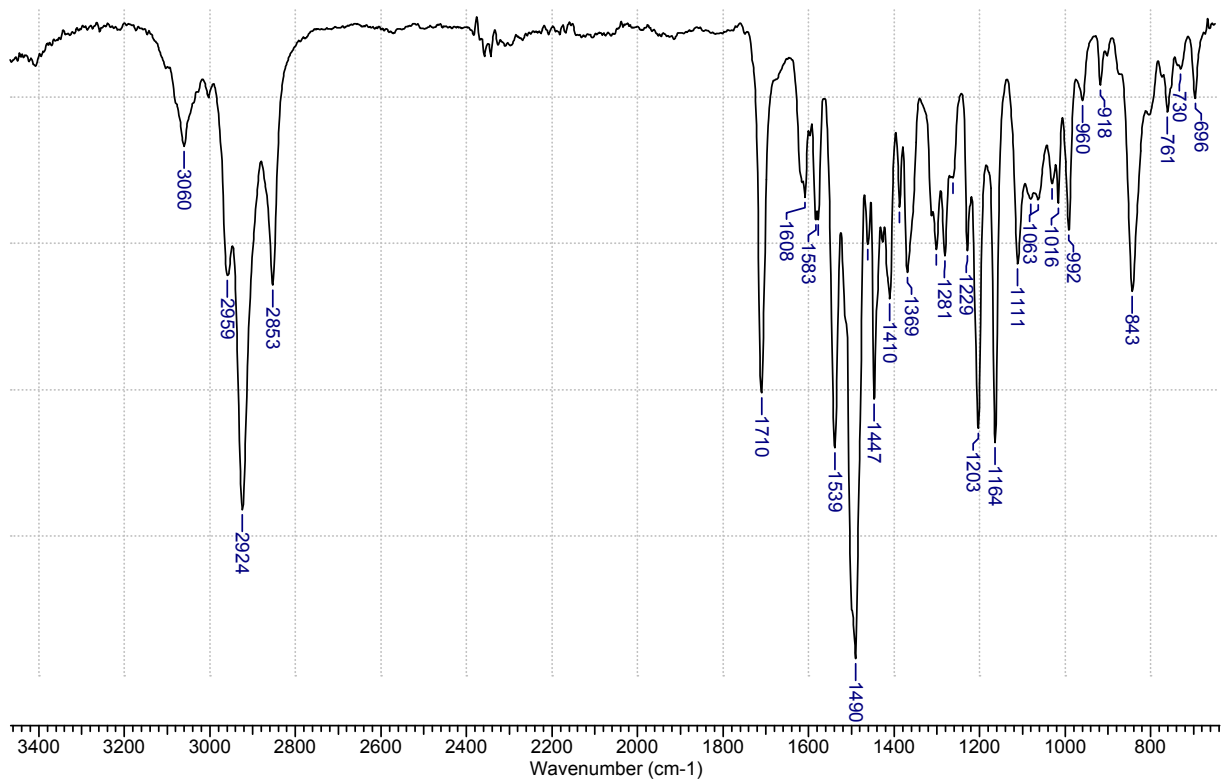


Fig. S12 FT-IR Spectrum of Ir-BD.

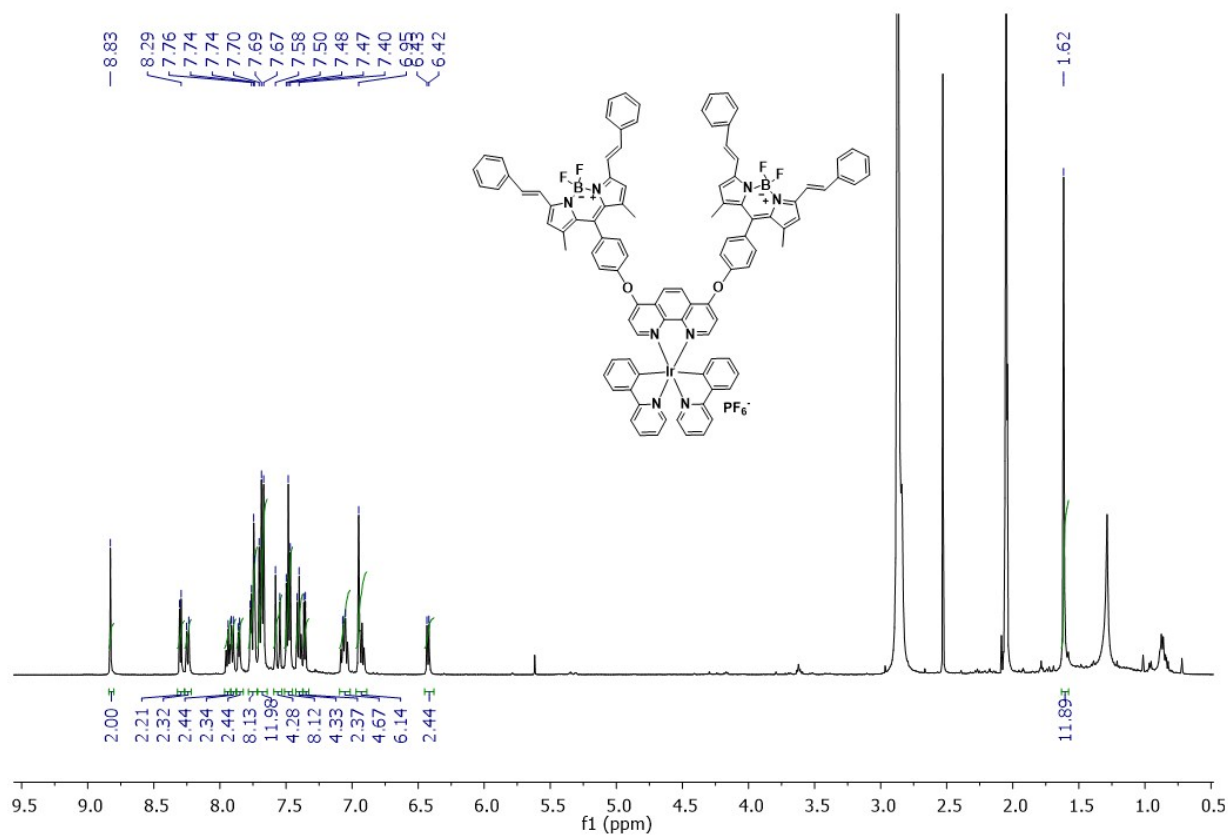


Fig. S13 ¹H-NMR spectrum of Ir-BD.

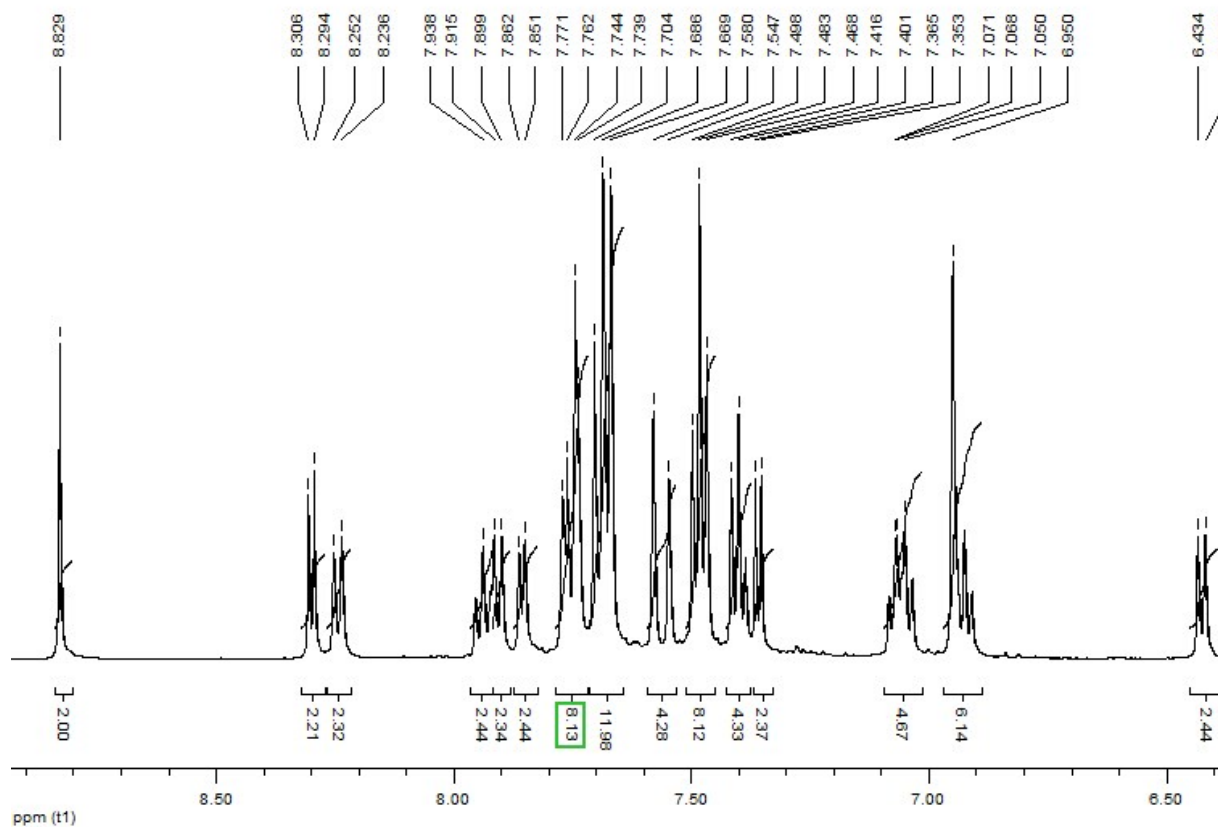


Fig. S14. Aromatic region of ¹H-NMR spectrum of Ir-BD.

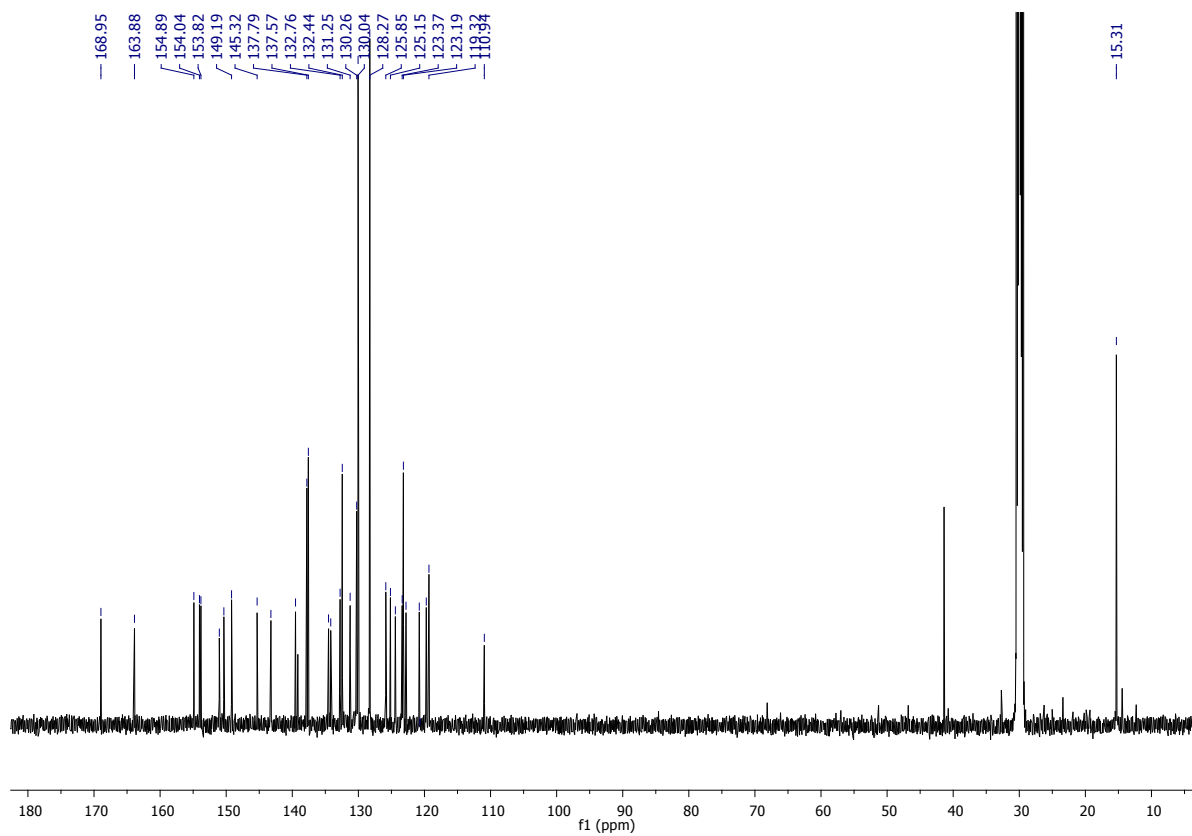


Fig. S15 ¹³C-NMR spectrum of Ir-BD.

Table S1. The selected bond and conformational parameters for **BD** and **3**

BD		3	
B1—F1	1.405 (4)	Ru1-N1	2.061 (4)
B1—F2	1.393 (4)	Ru1-N2	2.075 (4)
B1—N1	1.540 (4)	Ru1-N3	2.065 (4)
B1—N2	1.521 (4)	Ru1-N4	2.064 (4)
C1-C18	1.436 (4)	Ru1-N5	2.064 (4)
C3-C27	1.491 (5)	Ru1-N6	2.059 (4)
C5-C28	1.485 (4)	C3-Cl1	1702 (5)
C7-C26	1.492 (4)	C8- Cl2	1720 (5)
C9-C10	1.427 (4)	C17-C18	1.453 (7)
O1-C31	1.360 (3)	C27-C28	1.443(7)
O1-H1	0.877 (10)	N1-Ru1-N2	79.46 (15)
N1-C9	1.351 (4)	N2-Ru1-N6	97.03 (16)
N1-C6	1.392 (3)	N3-Ru1-N6	96.30 (16)
N2-C1	1.369 (4)	N5-Ru1-N6	78.62 (17)
N2-C4	1.390 (4)	N3-Ru1-N5	95.10 (16)
F2-B1-F1	107.6 (2)	N3-Ru1-N4	78.40 (17)
F1-B1-N2	110.6 (2)	N4-C18-C19	120.8 (5)
F1-N1-B1	109.0 (3)	N3-C17-C16	121.2 (5)
N2-B1-N1	107.6 (2)		
C1-C18-C19	123.2 (3)		
C4-C5-C6	120.7 (3)		
C4-N2-C1	107.9 (2)		
C6-N1-B1	124.8 (2)		
C5-C28-C29	121.0 (3)		
C9-C10-C11	124.9 (3)		
C6-C5-C28-C29	99.8 (3)		
C4-C5-C28-C33	105.7 (3)		
C4-C5-C28-C29	-77.8 (4)		
C6-C5-C28-C29	99.8 (3)		
C6-C5-C28-C33	-76.7 (4)		
C6-N1-C9-C10	-174.5 (3)		
F1-B1-N1-C9	65.7 (4)		
F1-B1-N1-C6	-119.2 (3)		

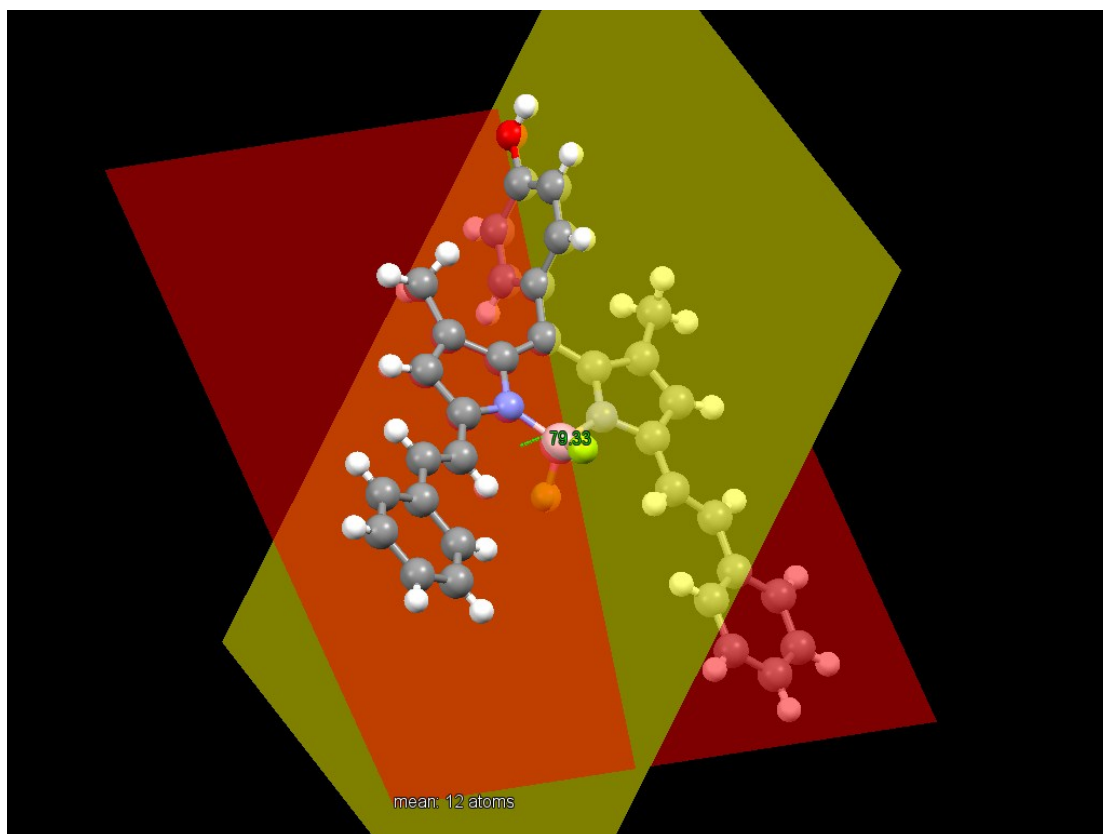


Fig. S16 The angle between the planes of BODIPY and phenol ring in BD.

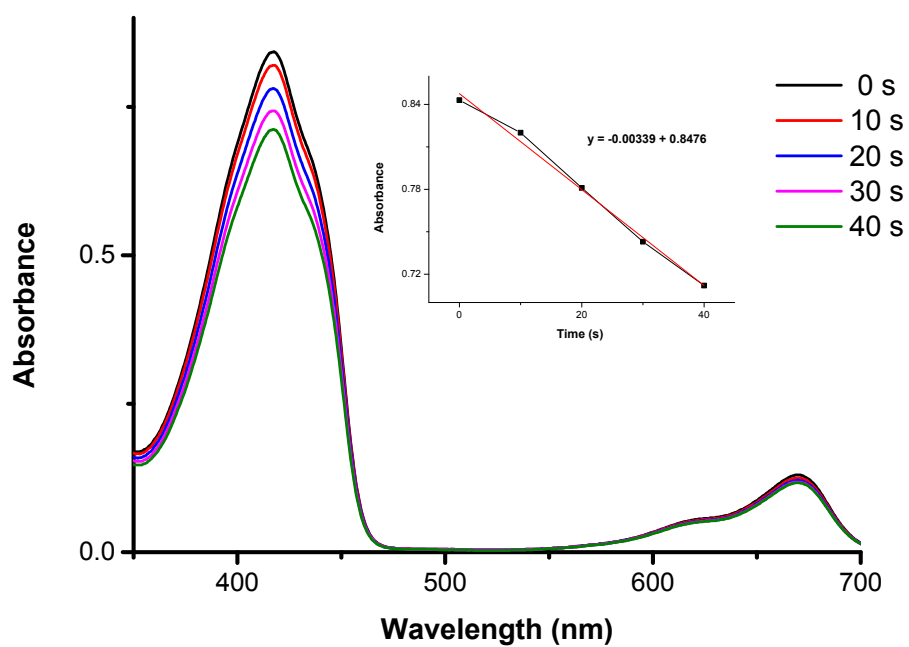


Fig. S17 UV-vis spectrum of methylene blue in DMSO.

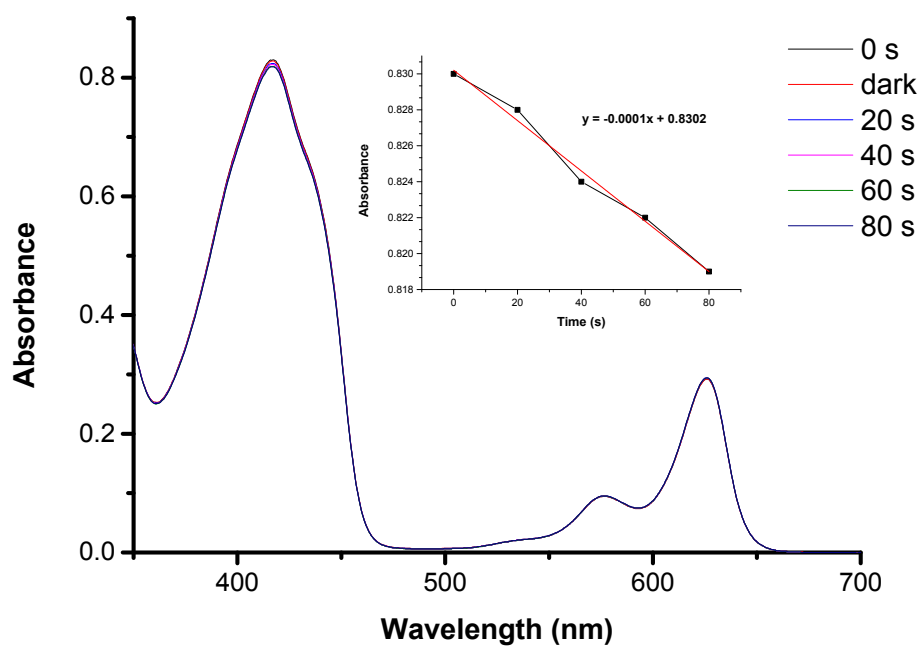


Fig. S18 UV-vis spectrum of BD in DMSO.

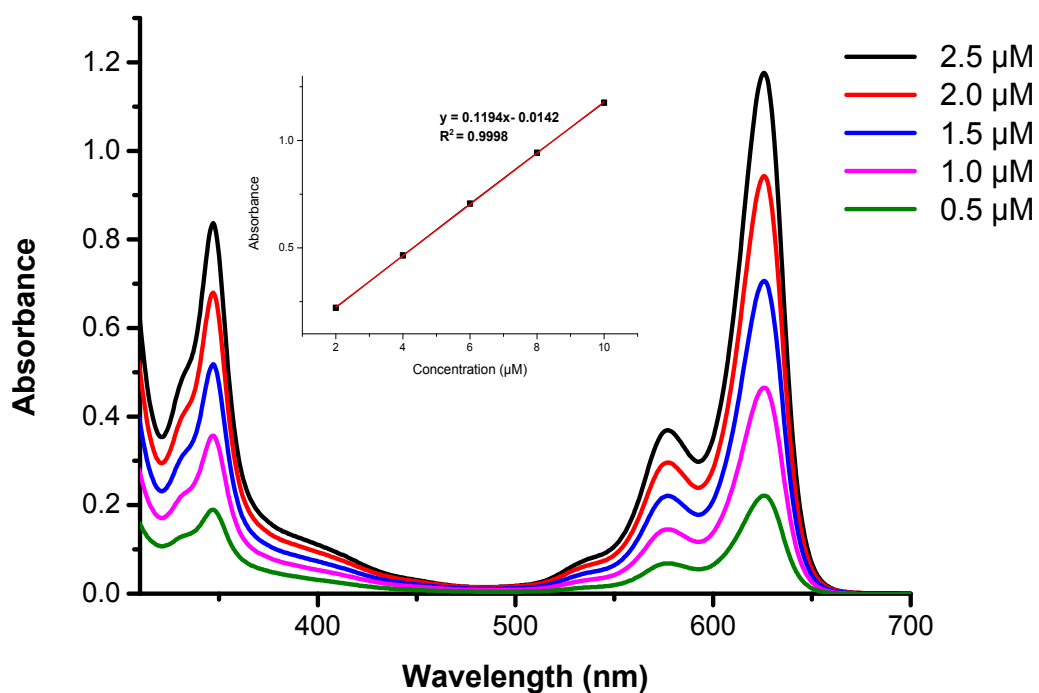


Fig. S19 UV-vis spectra of BD in DMSO at different concentrations between 2.5×10^{-6} M and 0.5×10^{-6} M.

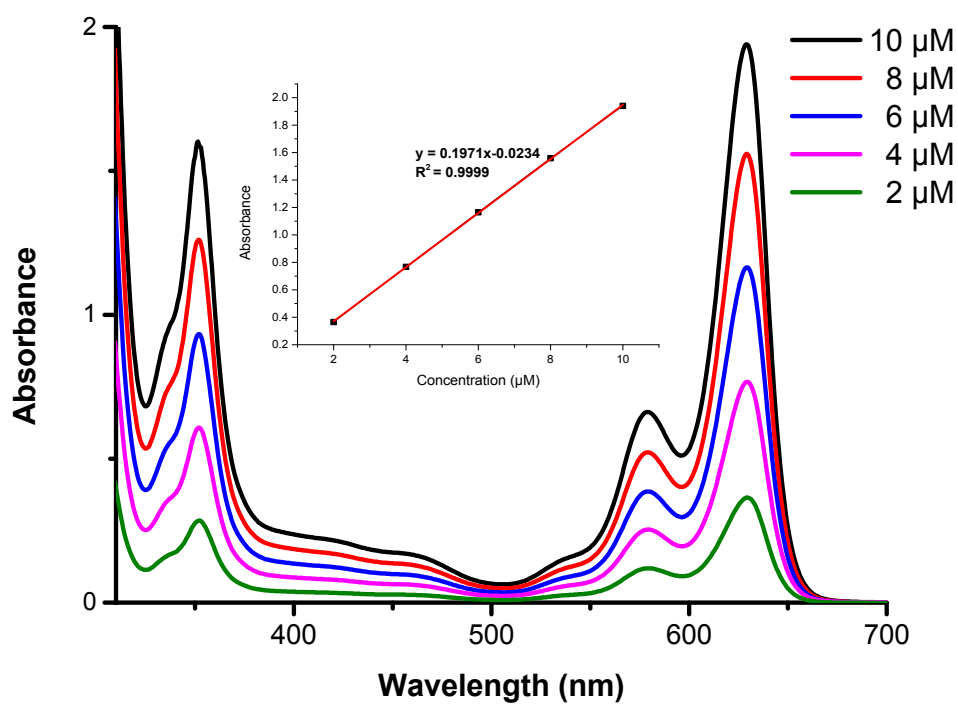


Fig. S20 UV-vis spectra of **Ru-BD** in DMSO at different concentrations between 2.5×10^{-6} M and 0.5×10^{-6} M.

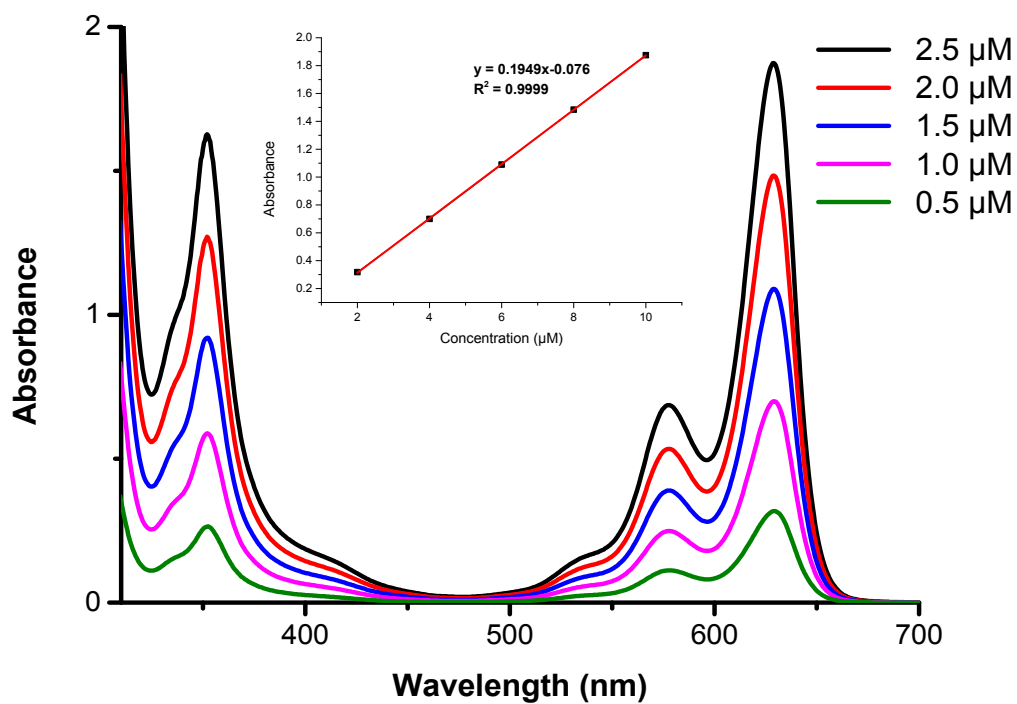


Fig. S21 UV-vis spectra of **Ir-BD** in DMSO at different concentrations between 2.5×10^{-6} M and 0.5×10^{-6} M.

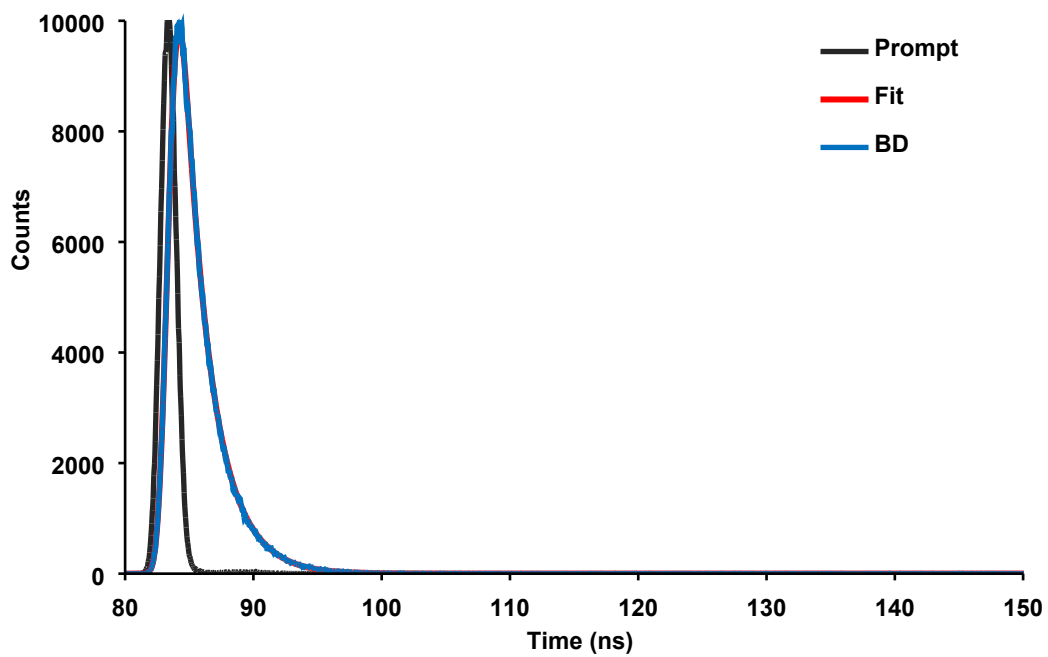


Fig. S22 Lifetime spectra of BD.

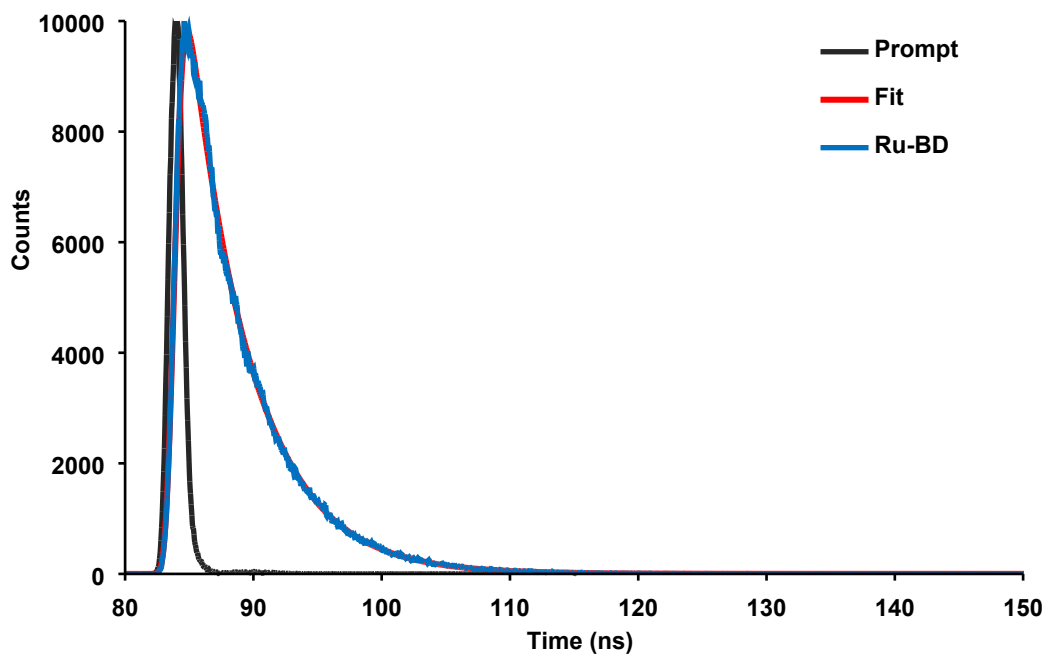


Fig. S23 Lifetime spectra of Ru-BD.

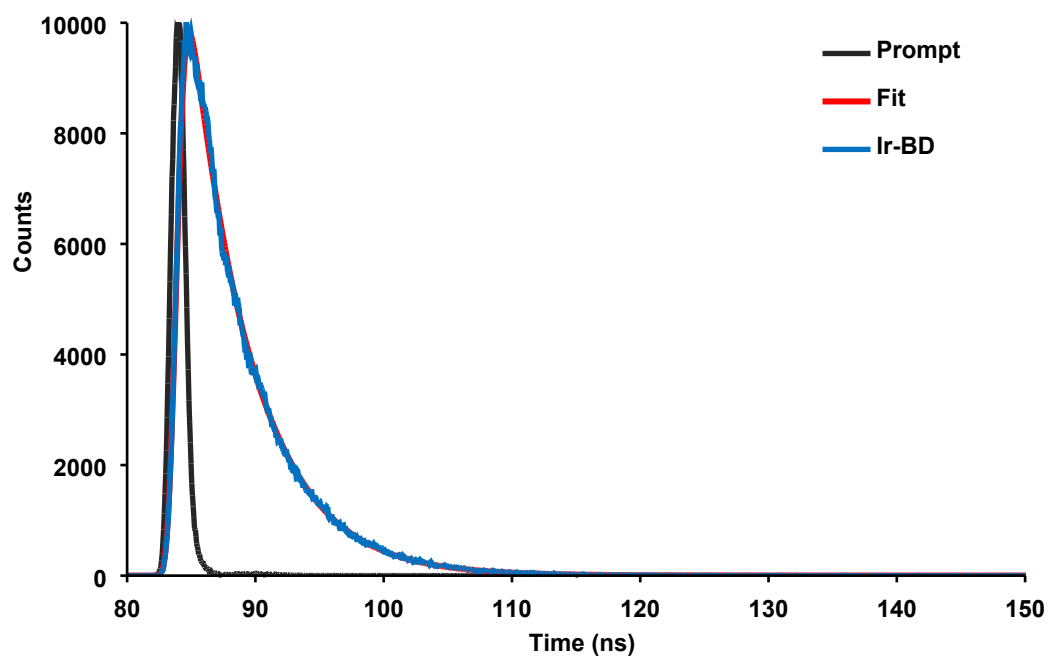


Fig. S24 Lifetime spectra of Ir-BD.