Supplementary Information

Benzothiazole-decorated iridium-based nano-photosensitizers for photodynamic therapy of cancer cells

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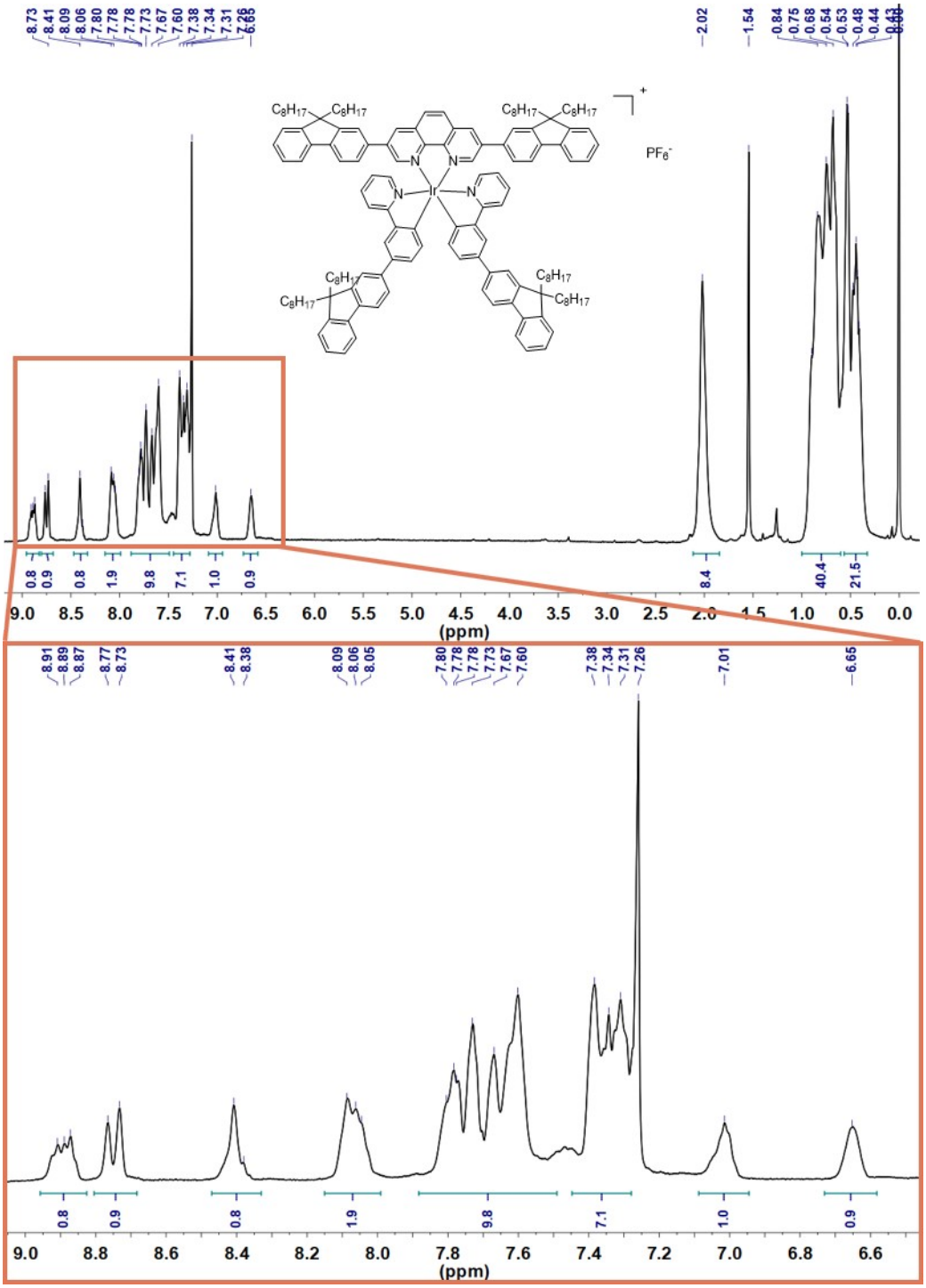

Fig. S1. ^{1}H NMR of **1**.

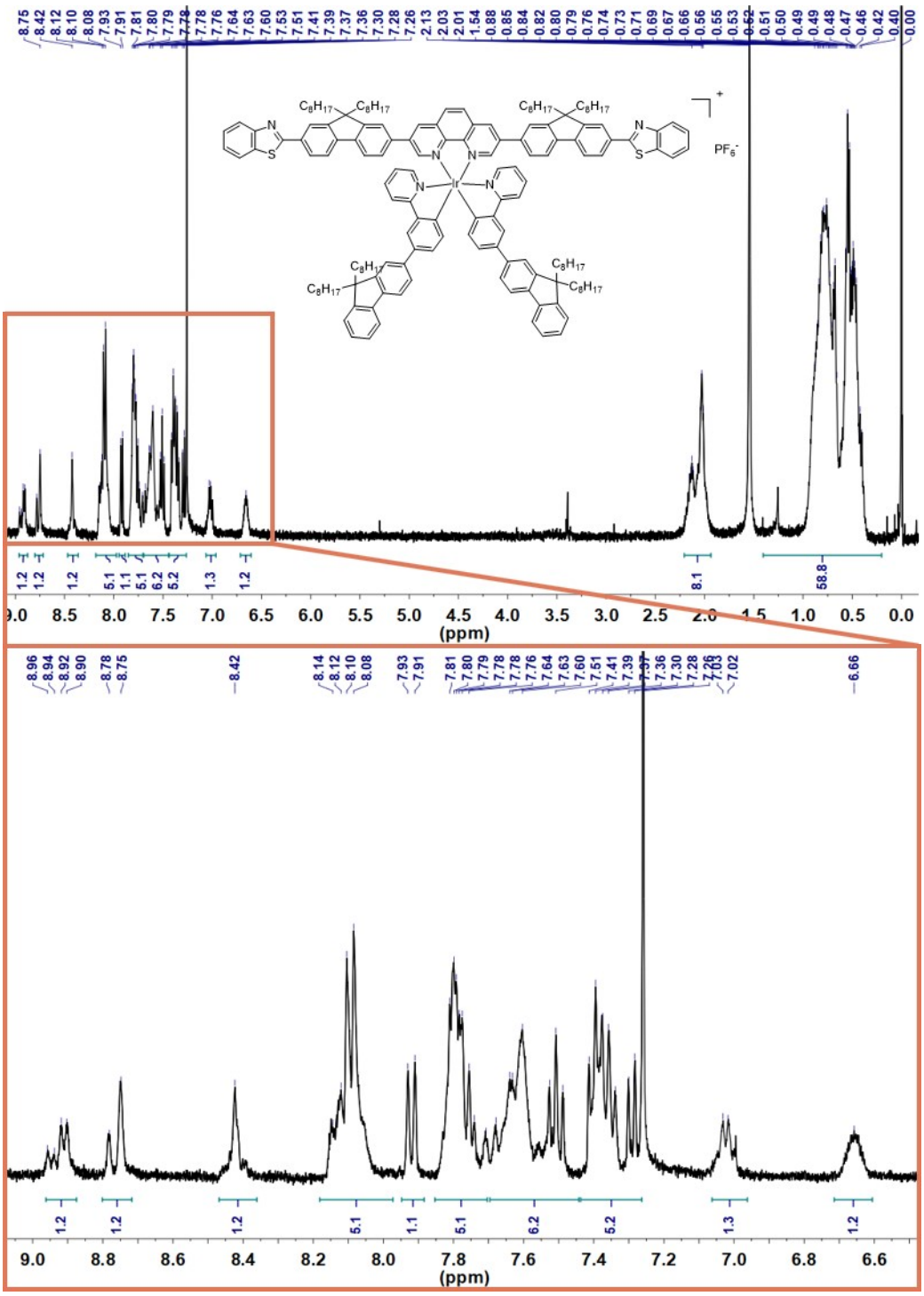

Fig. S2. ^{1}H NMR of **2**.

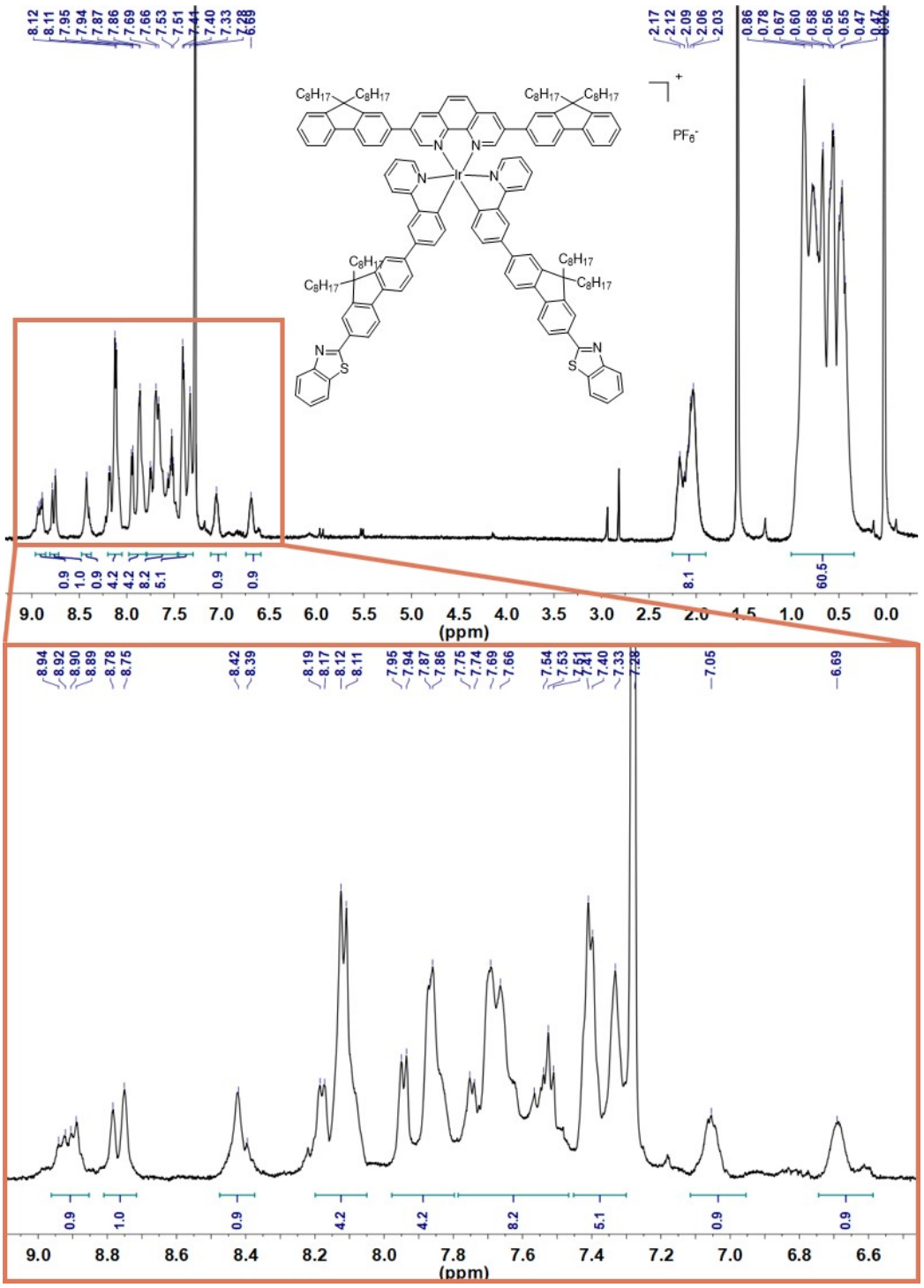

Fig. S3. ^{1}H NMR of **3**.

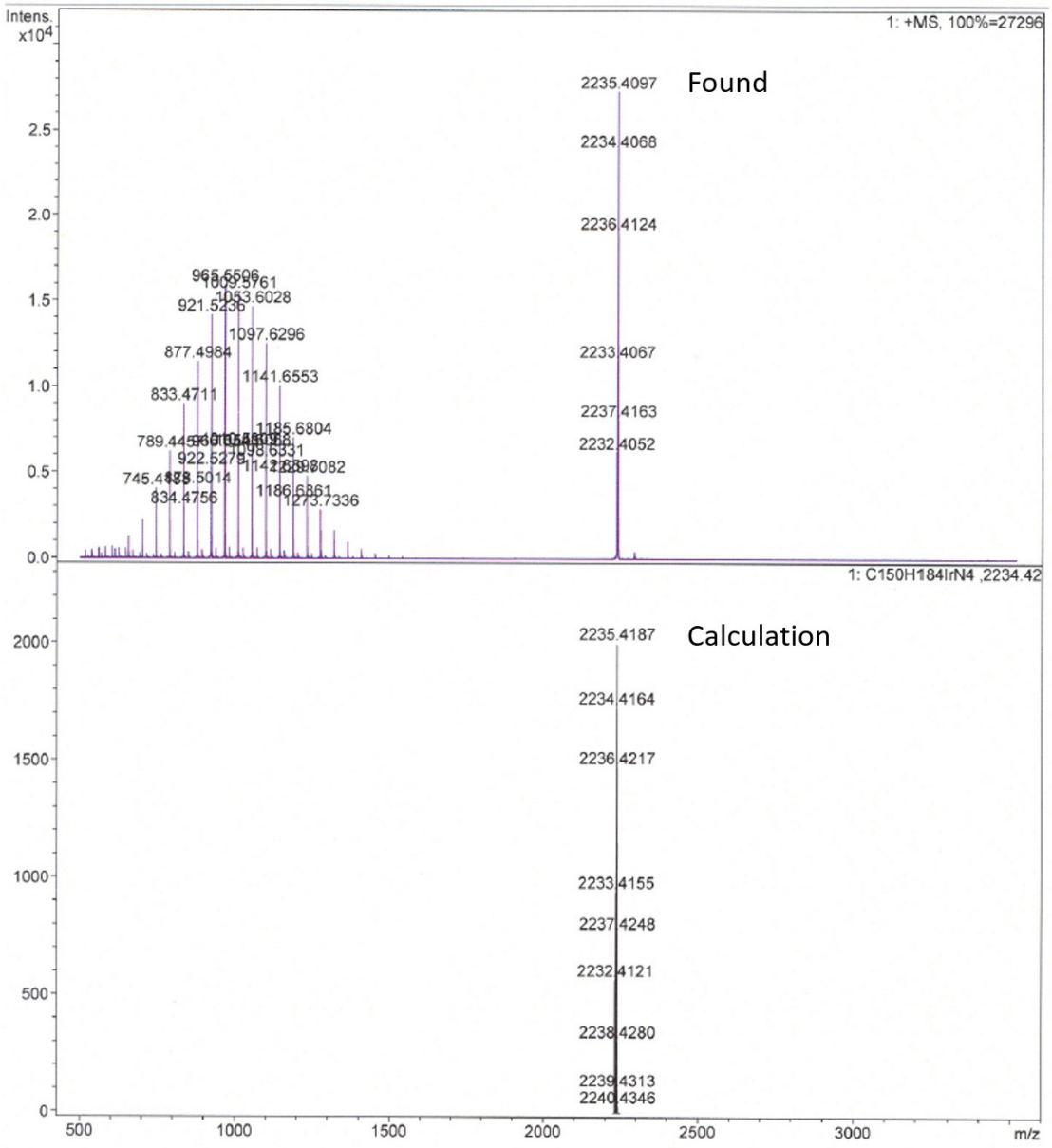

Fig. S4. HR-MS of **1**.

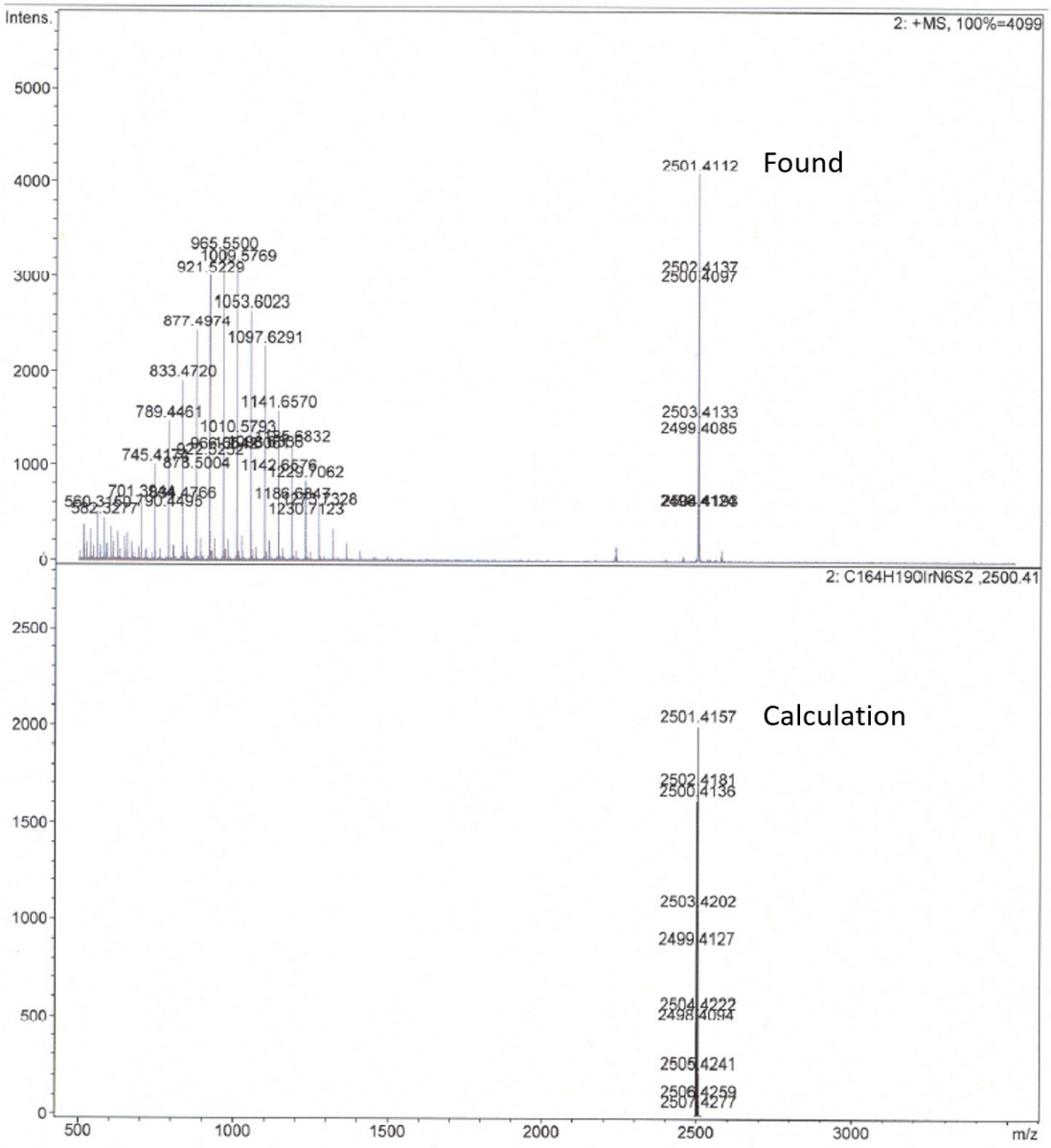

Fig. S5. HR-MS of **2**.

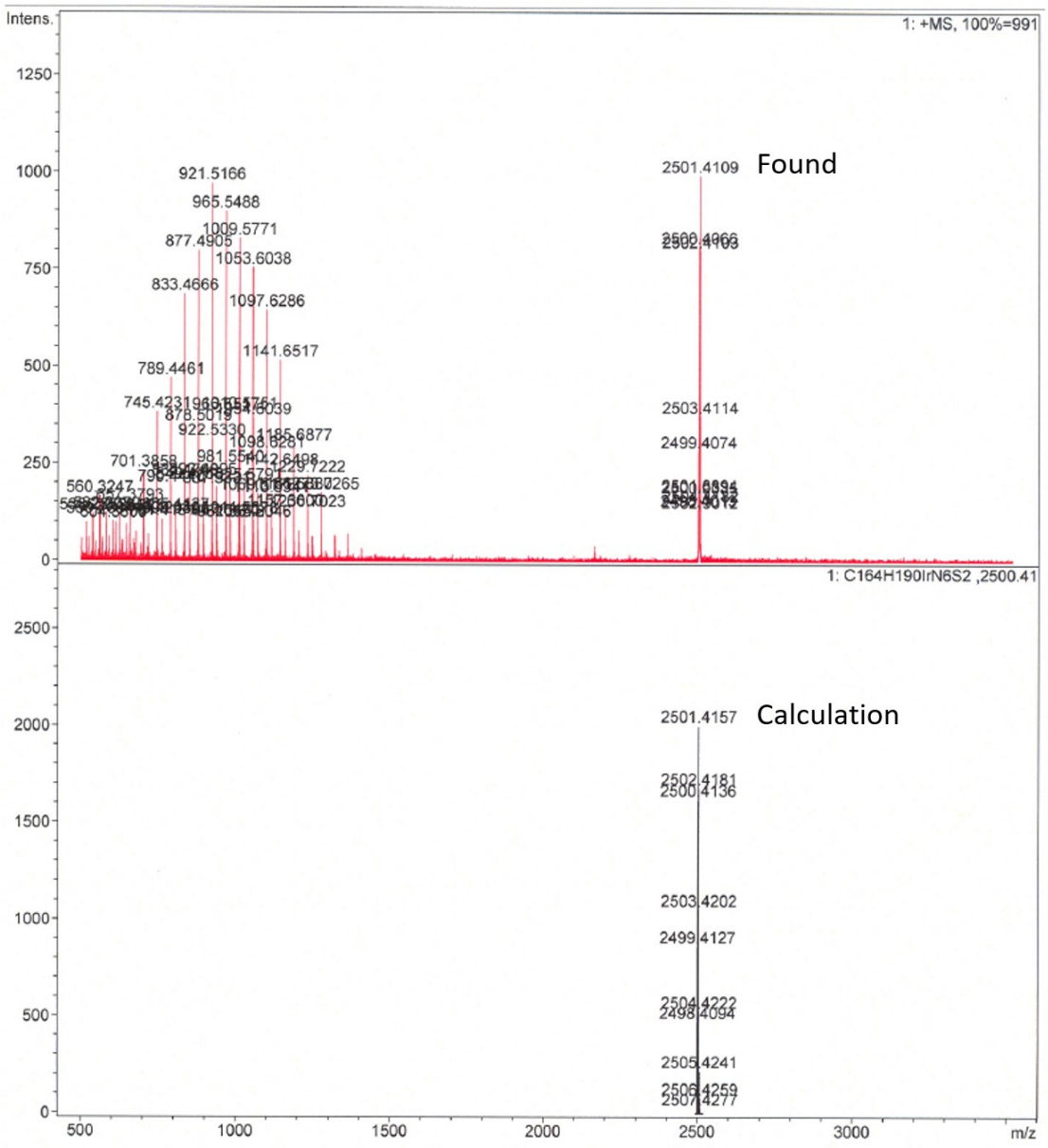

Fig. S6. HR-MS of **3**.

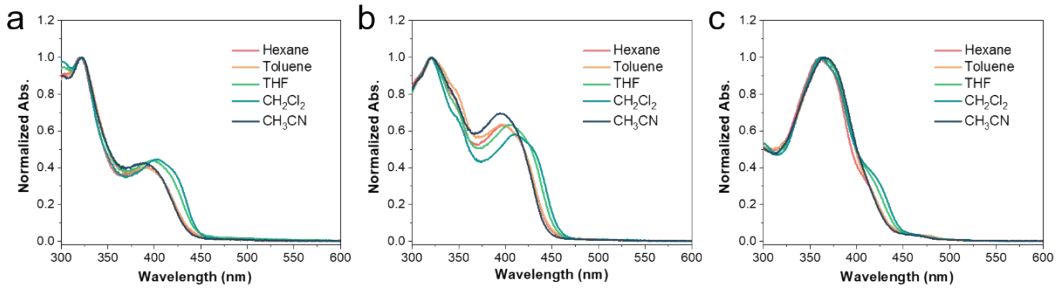

Fig. S7. Normalized absorption spectra of (a) **1**, (b) **2**, and (c) **3** in various solvents.

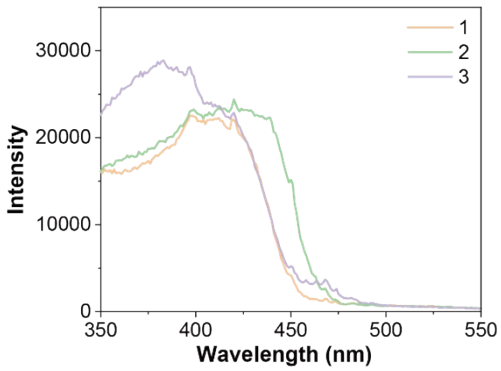

Fig. S8. Excitation spectra of complexes 1 – 3 in degassed CH_2Cl_2 (10 μM, maxima emission peak 603 nm for 1, 612 nm for 2, and 584 nm for 3).

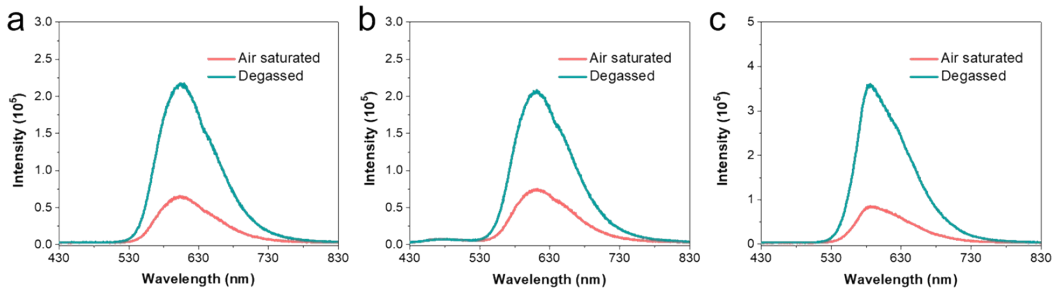

Fig. S9. Emission spectra of (a) **1**, (b) **2**, and (c) **3** in the air saturated or degassed CH_2Cl_2 solvent. (10 μM, λ_{ex} = 420 nm)

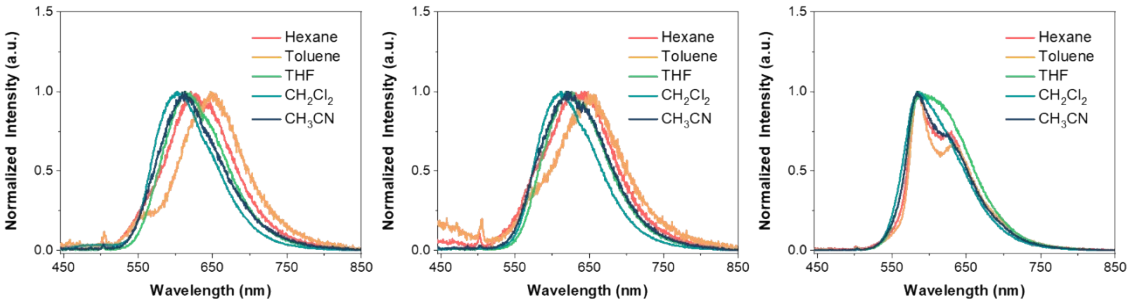

Fig. S10. Normalized emission spectra of (a) **1**, (b) **2**, and (c) **3** in various solvents. (λ_{ex} = 436 nm)

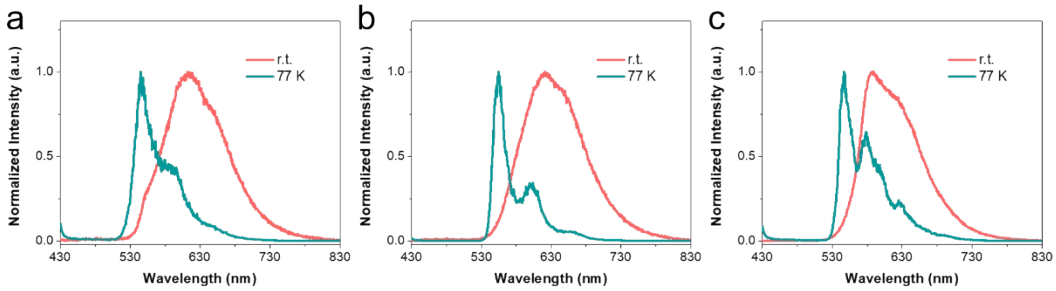

Fig. S11. Normalized emission spectra of (a) **1**, (b) **2**, and (c) **3** in BuCN solvent at room temperature or 77 K. (10 μM, λ_{ex} = 420 nm)

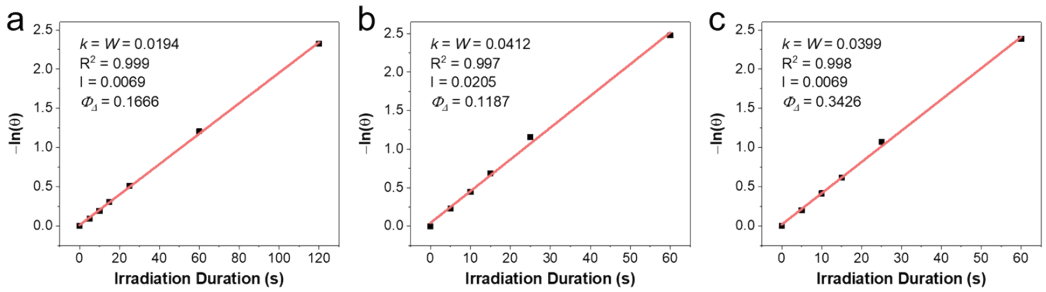

Fig. S12. Plotting and fitting absorbance decay of DPBF mixed with Ir(III) complex (a) **1**, (b) **2**, and (c) **3** in toluene under light irradiation (532 nm, 100 mW cm^{-2}). *k*: fitted slope value; *I*: sample absorption rate at 532 nm.

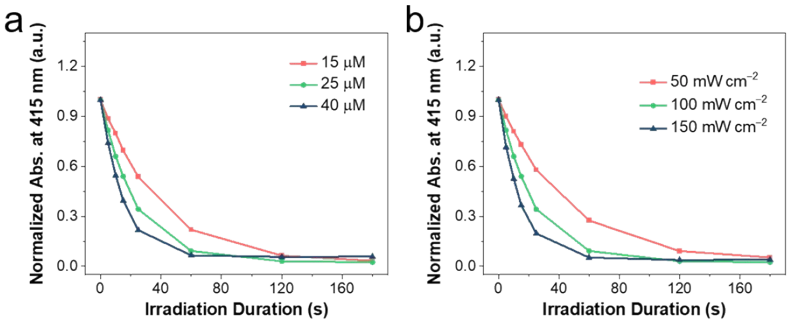

Fig. S13. (a) concentration- and (b) light power density-dependent $^1O_2$ generation of complex 3.

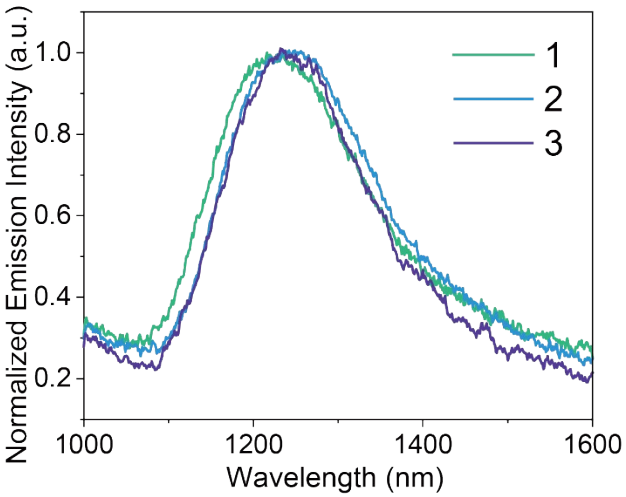

Fig. S14. Normalized singlet-oxygen emission spectra of complexes 1 – 3 in CH_2Cl_2 (10 μM, λ_{ex} = 420 nm).

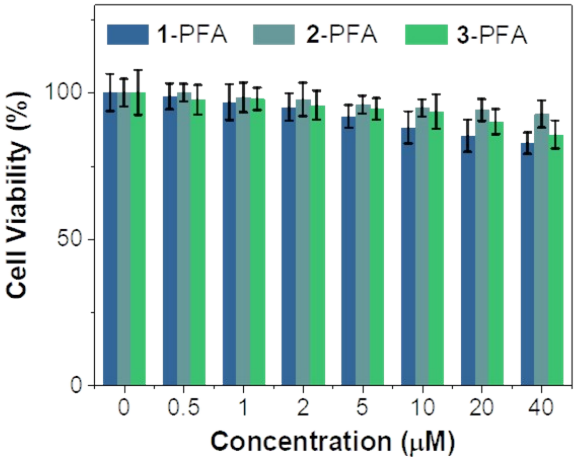

Fig. S15. 4T1.2 cell viability after 48 h of incubation with **1**-PFA, **2**-PFA and **3**-PFA.

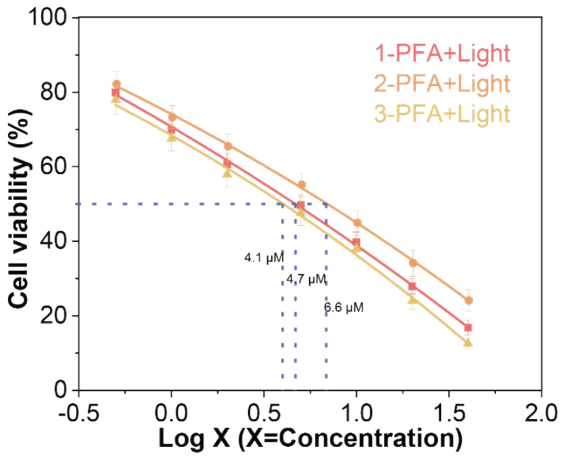

Fig. S16. The value of IC_{50} with 1-PFA – 3-PFA.

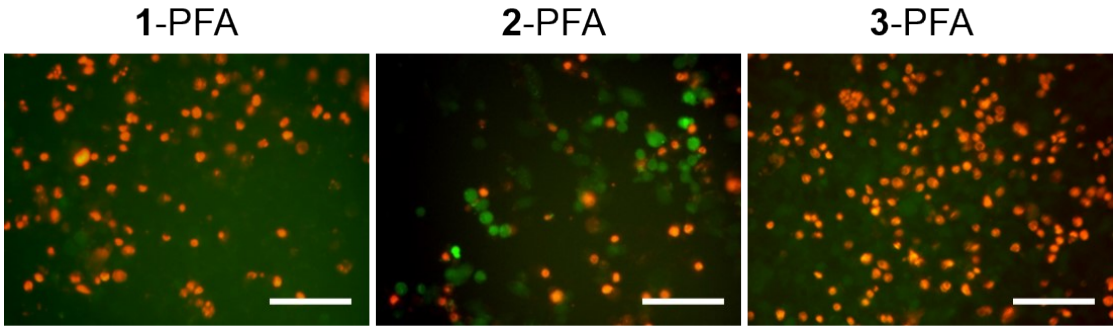

Fig. S17. Live and dead cells co-staining of 4T1.2 cells after PDT with **1**-PFA, **2**-PFA and **3**-PFA.

	λ_{em}/nm (τ_{em}/μs); Φ_{em}[a]				
	Hexane[b]	toluene	CH_2Cl_2	THF	CH_3CN
1	621 (0.32); 0.02	650 (0.15); 0.02	603 (0.82); 0.05	614 (0.51); 0.04	613 (0.22); 0.02
2	640 (0.37); 0.01	654 (0.13); 0.02	612 (0.88); 0.05	622 (0.47); 0.03	622 (0.36); 0.02
3	585 (3.96), 630 (3.62); 0.02	584 (4.20), 633 (3.43); 0.02	584 (1.21); 0.05	587 (0.74); 0.03	585 (0.65), 626 (0.57); 0.02

Table S1. Emission properties of **1** – **3** in different polarity solvents.

[a]Degassed $[Ru(bpy)_3]Cl_2$ aqueous solution (λ_{ex} = 436 nm, Φ_{em} = 0.57) was used for reference substance. [b]With 5% CH_2Cl_2.

Table S2 Singlet-oxygen quantum yields of various photosensitizers.

	Compound	Meatal center	λ_{exc} (nm)	$^1O_2$ (Φ_Δ)
1	1 in this work	Ir (III)	532	0.17
2	2 in this work	Ir (III)	532	0.12
3	3 in this work	Ir (III)	532	0.34
4	C14-IP2000[1]	Ir (III)	532	0.23
5	Ir2[2]	Ir (III)	532	0.27
6	BODIPY-Ir[3]	Ir (III)	500	0.35
7	Ir-OH[4]	Ir (III)	405	0.31
8	Ir-B(OH)$_2$[4]	Ir (III)	405	0.32
9	Ir[5]	Ir (III)	405	0.46
10	Complex 1[6]	Ir (III)	405	0.42
11	Complex 2[6]	Ir (III)	405	0.40

Reference

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