Electronic Supplementary Information

BSA-encapsulated cyclometalated iridium complexes as nano-photosensitizers for photodynamic therapy of tumor cells

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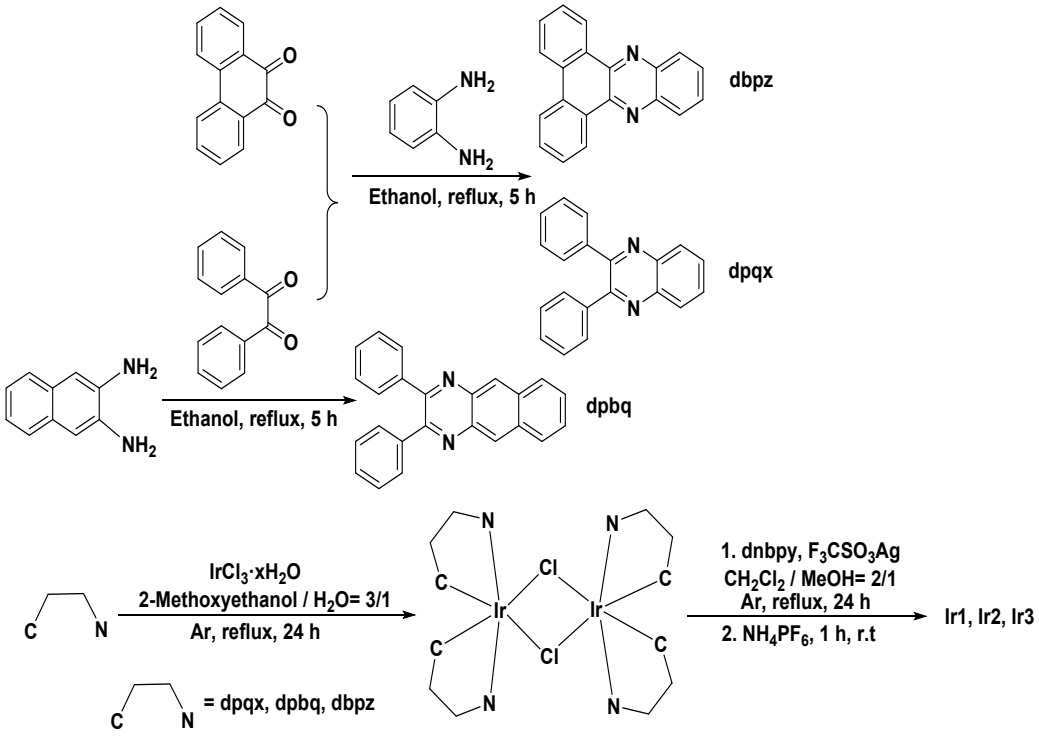

Fig. S1. Synthetic route of Ir1, Ir2, and Ir3.

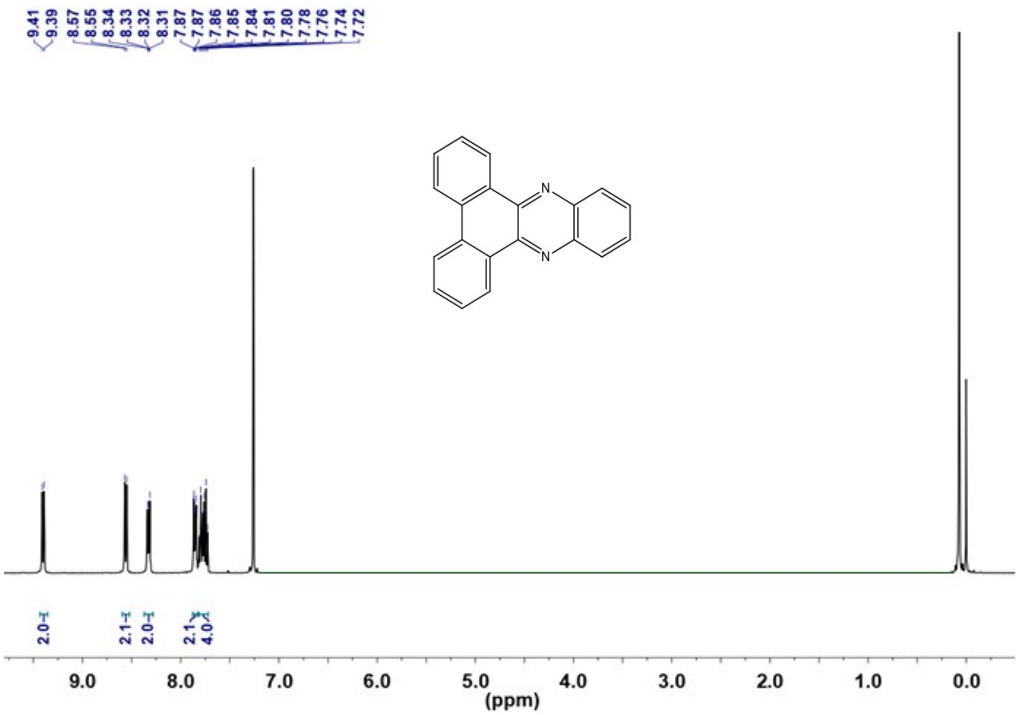

Fig. S2. ^{1}H-NMR of dbpz.

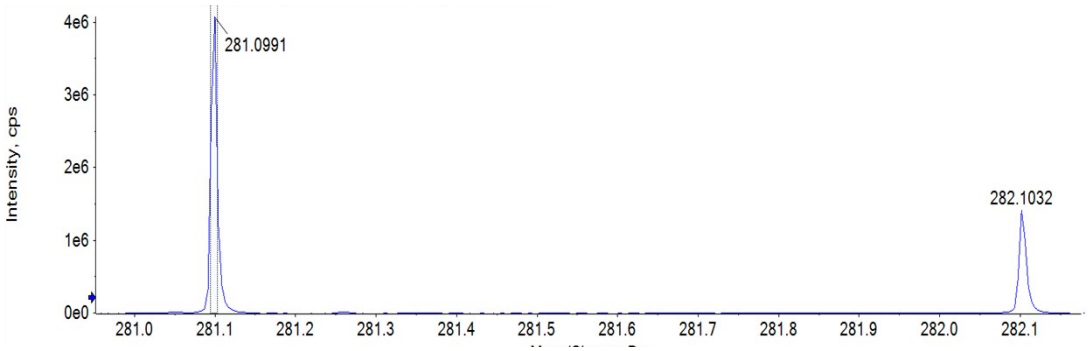

Fig. S3. HR-MS of dbpz.

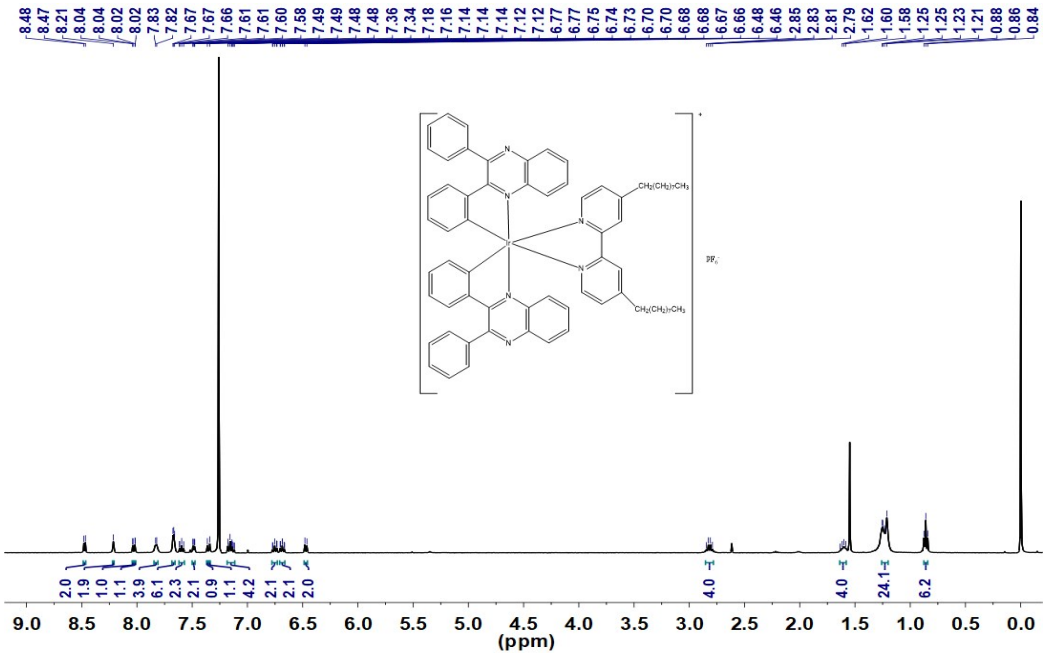

Fig. S4. ^{1}H-NMR of Ir1.

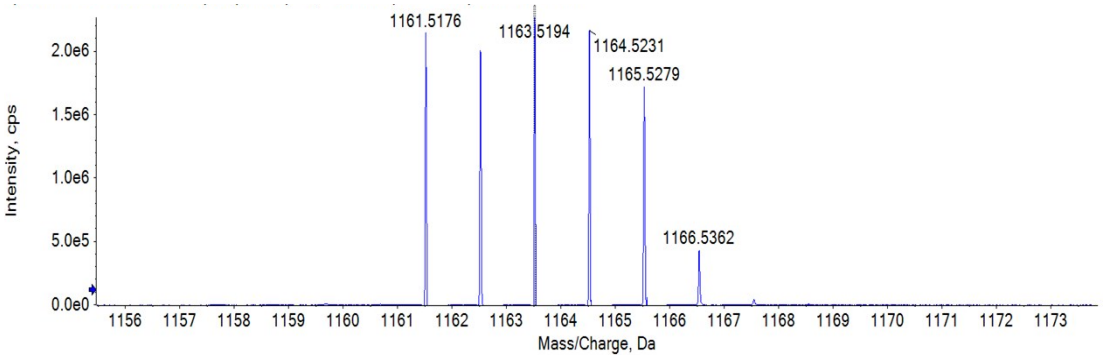

Fig. S5. HR-MS of Ir1.

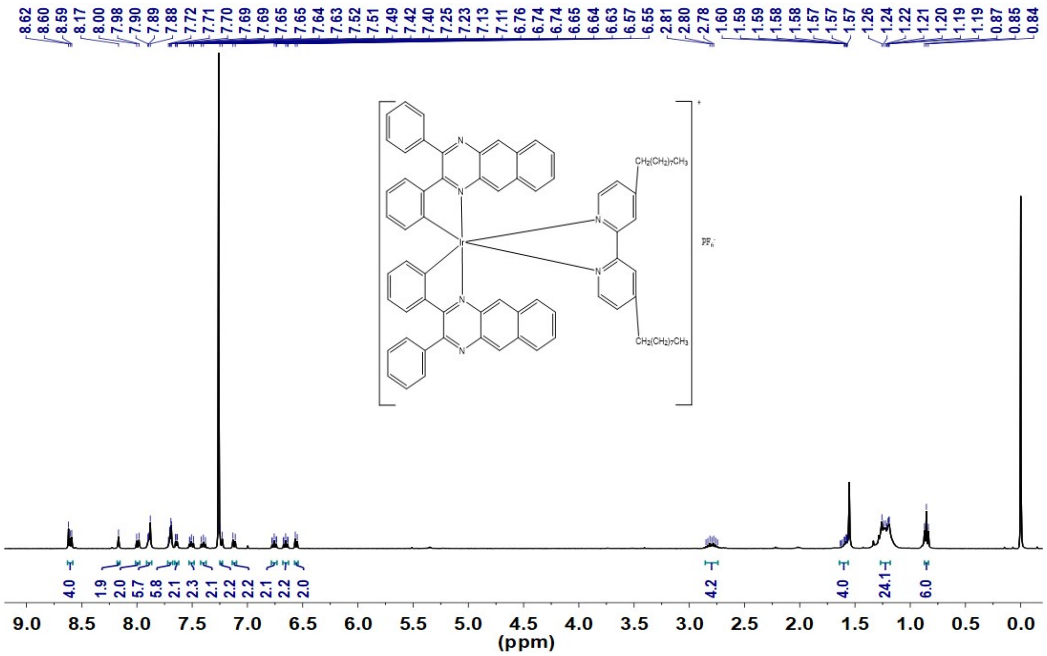

Fig. S6. [1]H-NMR of Ir2.

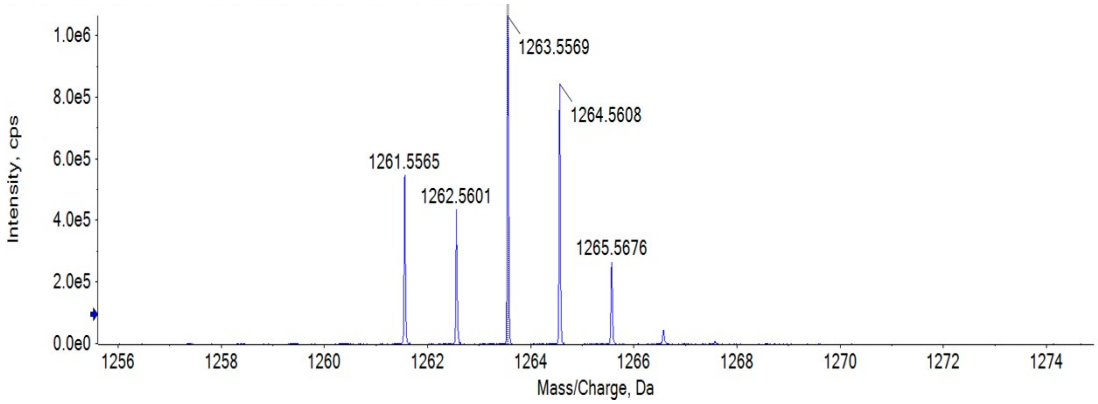

Fig. S7. HR-MS of Ir2.

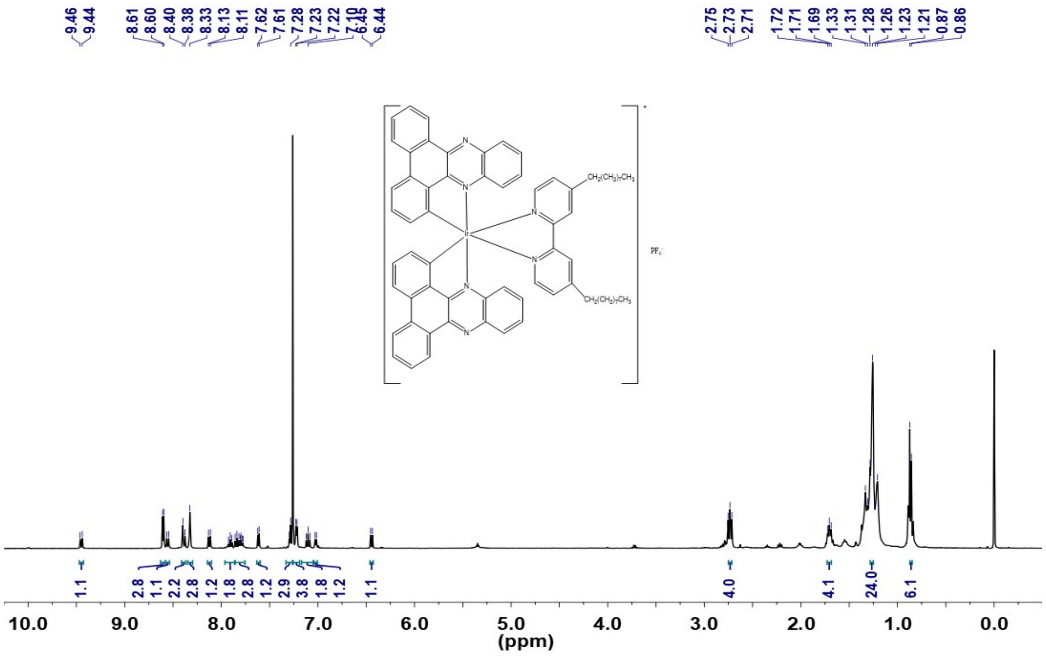

Fig. S8. ^{1}H-NMR of Ir3.

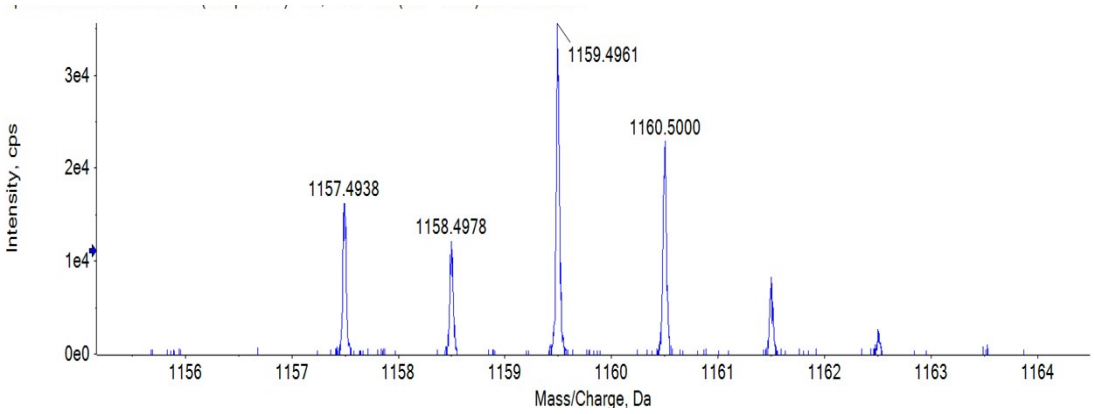

Fig. S9. HR-MS of Ir3.

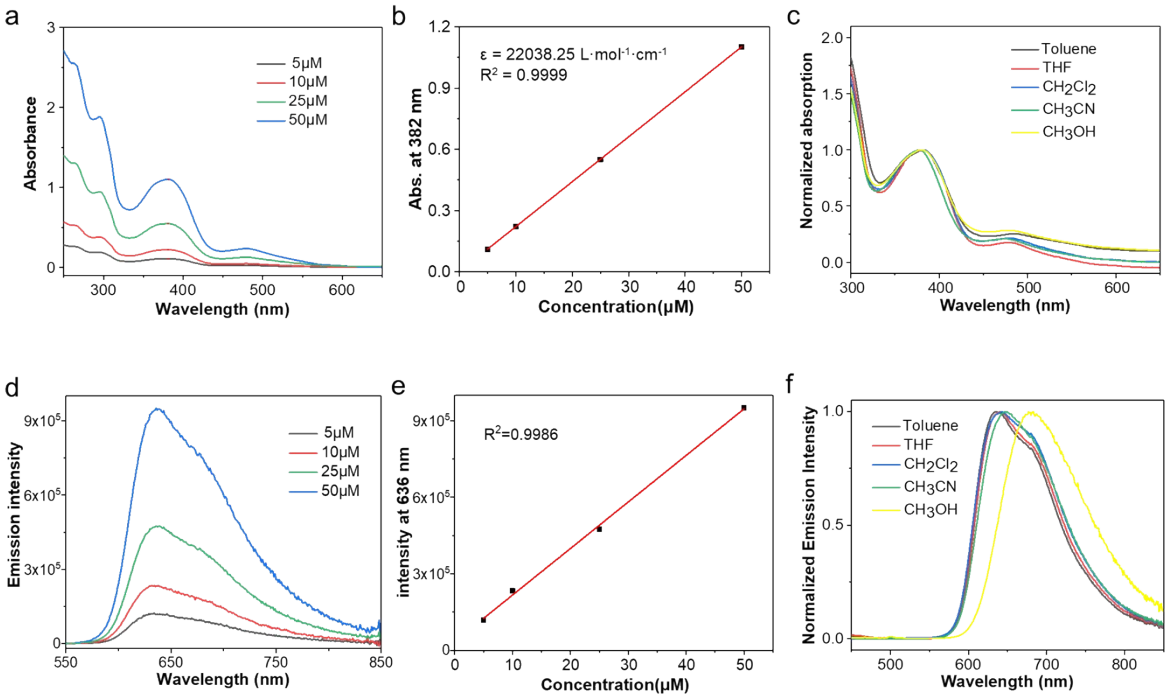

Fig. S10. (a) Absorption spectra of Ir1 in CH_2Cl_2 at various concentration, (b) absorbance linear fitting of Ir1 at 382 nm in CH_2Cl_2 at different concentrations, (c) normalized absorption spectra of Ir1 in different solvents, (d) emission intensity of Ir1 in CH_2Cl_2 at various concentration, (e) intensity-concentration linear fitting at 636 nm, (f) normalized emission intensity of Ir1 in different solvents (λ_{ex} = 436 nm).

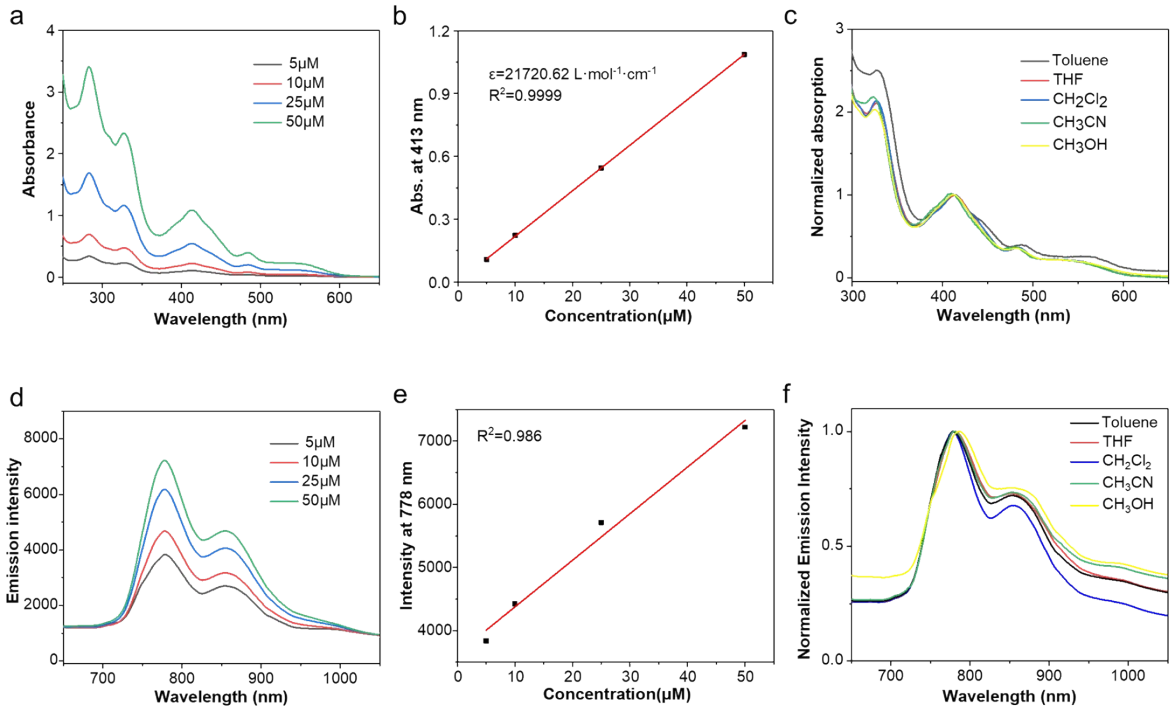

Fig. S11. (a) Absorption spectra of Ir2 in CH_2Cl_2 at various concentration, (b) absorbance linear fitting of Ir1 at 413 nm in CH_2Cl_2 at different concentrations, (c) normalized absorption spectra of Ir2 in different solvents, (d) emission intensity of Ir2 in CH_2Cl_2 at various concentration, (e) intensity-concentration linear fitting at 778 nm, (f) normalized emission intensity of Ir2 in different solvents (λ_{ex} = 532 nm).

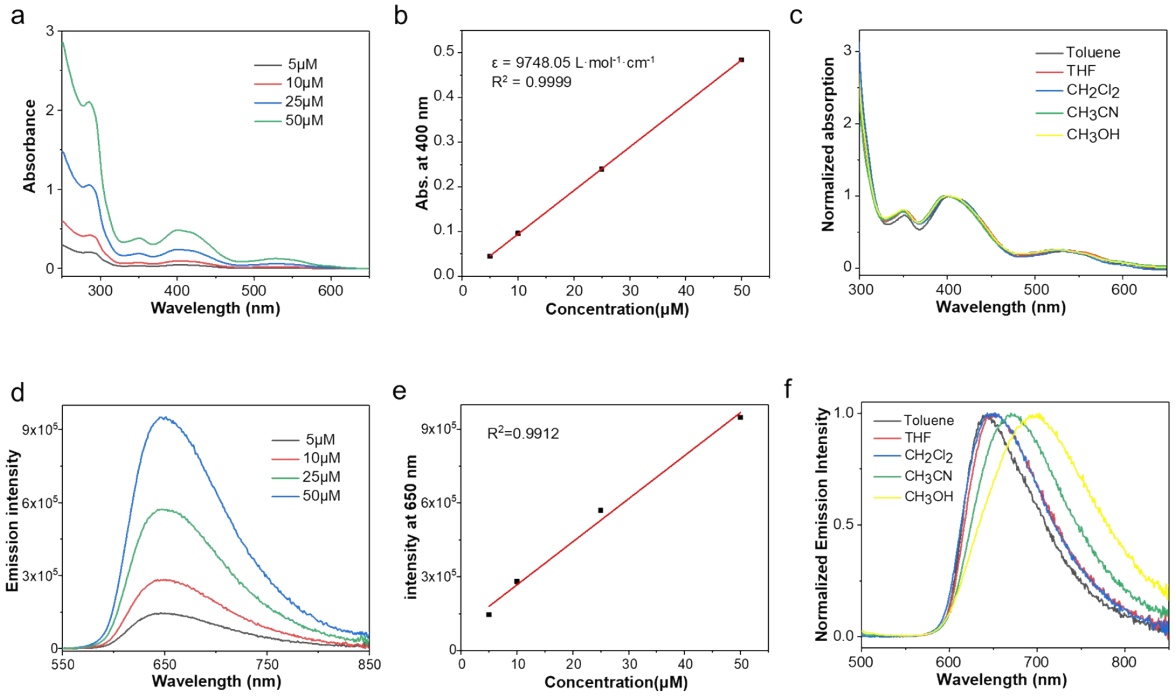

Fig. S12. (a) Absorption spectra of Ir3 in CH_2Cl_2 at various concentration, (b) absorbance linear fitting of Ir3 at 400 nm in CH_2Cl_2 at different concentrations, (c) normalized absorption spectra of Ir3 in different solvents, (d) emission intensity of Ir3 in CH_2Cl_2 at various concentration, (e) intensity-concentration linear fitting at 650 nm, (f) normalized emission intensity of Ir3 in different solvents (λ_{ex} = 436 nm).

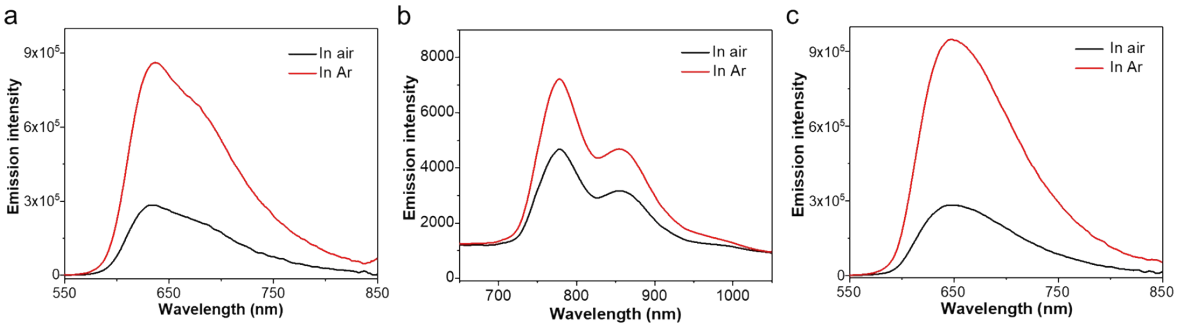

Fig. S13. Emission intensity of (a) Ir1 (λ_{ex} = 436 nm), (b) Ir2 (λ_{ex} = 532 nm) and (c) Ir3 (λ_{ex} = 436 nm) in CH_2Cl_2 under air or Argon (Ar) atmosphere.

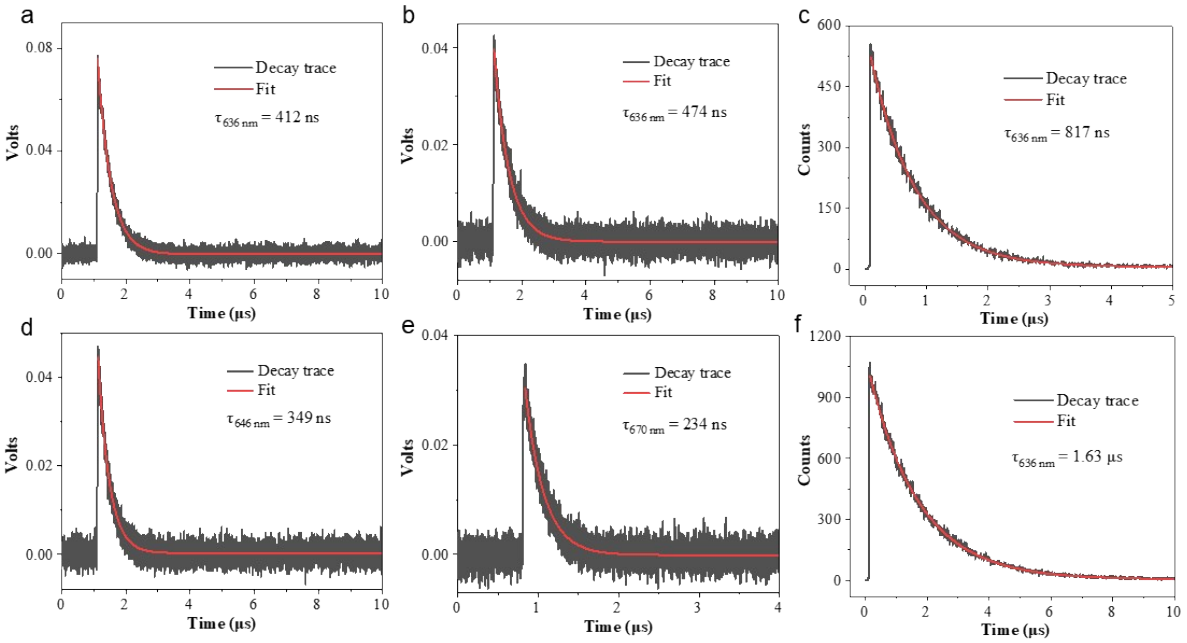

Fig. S14. Emission lifetime of Ir1 (a) at 636 nm in toluene, (b) at 636 nm in THF, (c) at 636 nm in CH_2Cl_2, (d) at 646 nm in CH_3CN, (e) at 670 nm in CH_3OH, (f) at 636 nm in degassed CH_2Cl_2 (λ_{ex} = 355 nm).

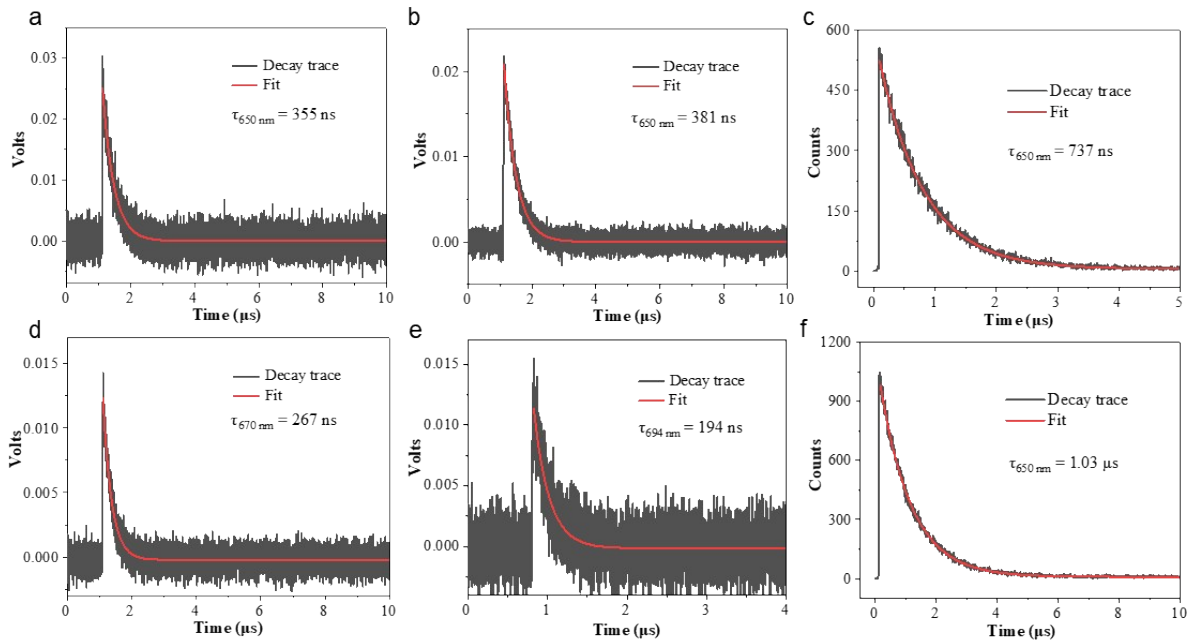

Fig. S15. Emission lifetime of Ir3 (a) at 650 nm in toluene, (b) at 650 nm in THF, (c) at 650 nm in CH_2Cl_2, (d) at 670 nm in CH_3CN, (e) at 694 nm in CH_3OH, (f) at 650 nm in degassed CH_2Cl_2 (λ_{ex} = 355 nm).

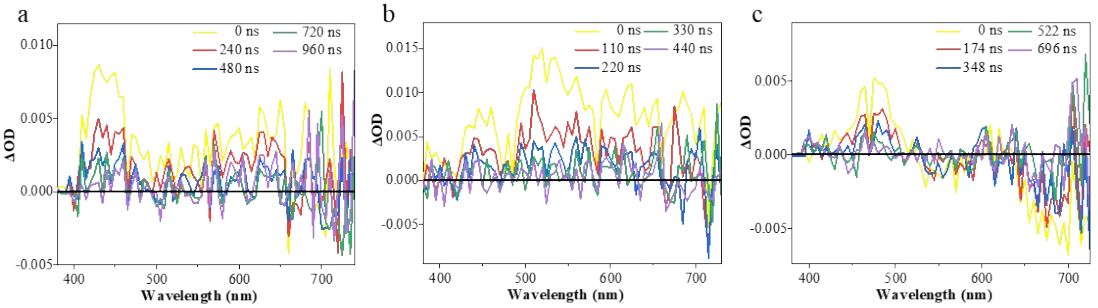

Fig. S16. Transient absorption spectra of (a) Ir1, (b) Ir2 and (c) Ir3 in deaerated CH_3CN, λ_{ex} = 355 nm.

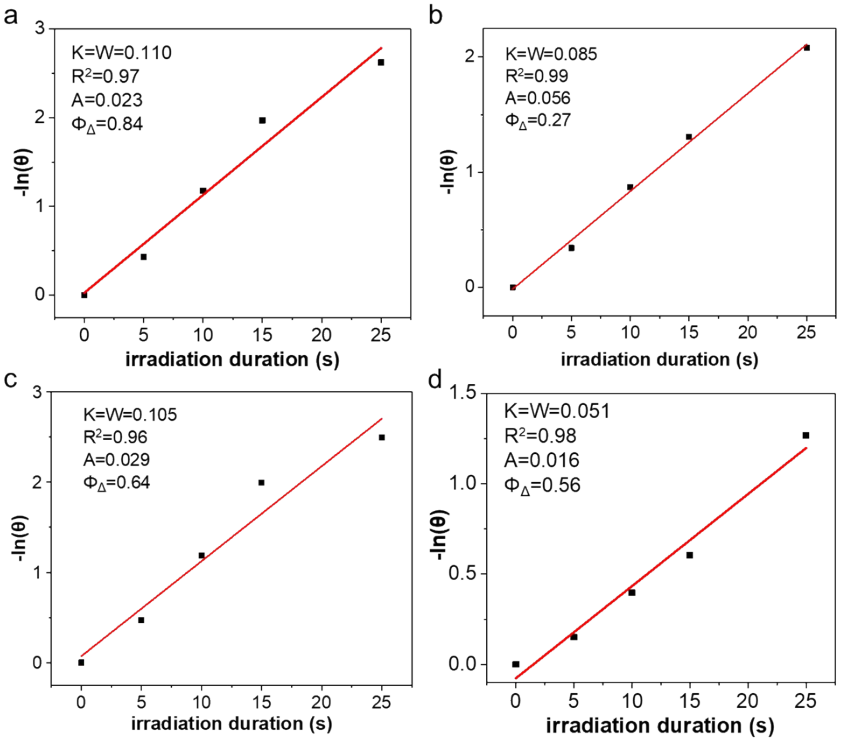

Fig. S17. The negative logarithm of the normalized absorbance changes at 410 nm with the irradiation time and the corresponding fitting line, (a) Ir1 + DPBF, (b) Ir2 + DPBF, (c) Ir3 + DPBF, and (d) $[Ru(bpy)_3]Cl_2$ + DPBF under 532 nm light irradiation (50 mW cm^{-2}).

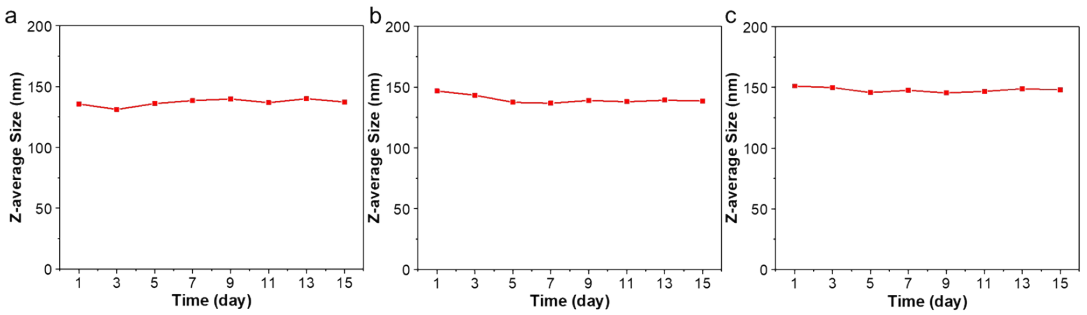

Fig. S18. Time-dependent hydrate particle size of (a) Ir1@BSA, (b) Ir2@BSA, and (c) Ir3@BSA for 15 days.

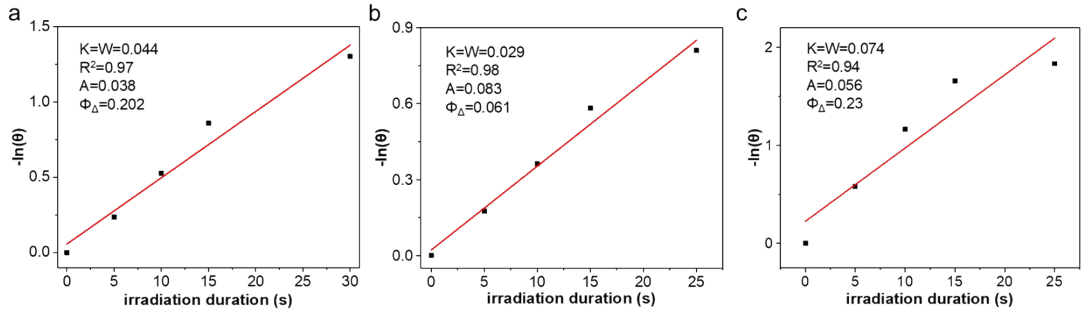

Fig. S19. The negative logarithm of the normalized absorbance changes at 415 nm with the irradiation time and the corresponding fitting line, (a) Ir1@BSA + DPBF, (b) Ir2@BSA+ DPBF, and (c) Ir3@BSA + DPBF under 532 nm light irradiation (50 mW cm^{-2}).

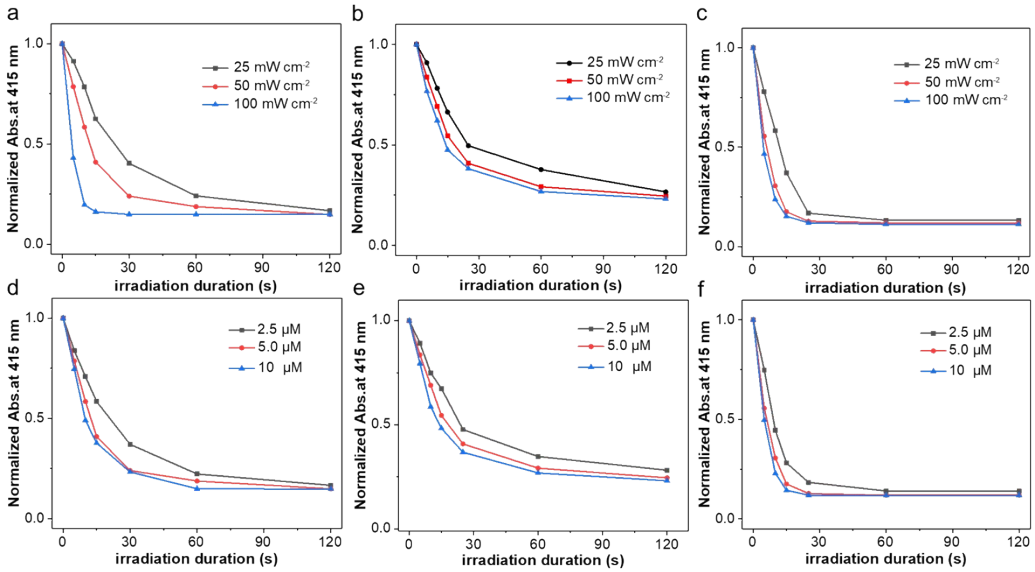

Fig. S20. Time-dependent absorbance plot at 415 nm of (a) Ir1@BSA + DPBF, (b) Ir2@BSA + DPBF, and (c) Ir3@BSA + DPBF under various laser power density or under various concentration of (d) Ir1@BSA, (e) Ir2@BSA, and (f) Ir3@BSA.

Table S1. Emission quantum yield (Φ_{em}) of Ir1 and Ir3 in different solvents calculated by the integrating sphere method (λ_{ex} = 532 nm)

Solvents	Toluene	THF	CH_2Cl_2	Degassed CH_2Cl_2	CH_3CN	CH_3OH
Ir1	0.146	0.179	0.176	0.336	0.081	0.054
Ir3	0.078	0.081	0.182	0.474	0.075	0.011