Supplementary Materials: Photophysical and Biological Properties of Iridium Tetrazolato Complexes Functionalised with Fatty Acid Chains

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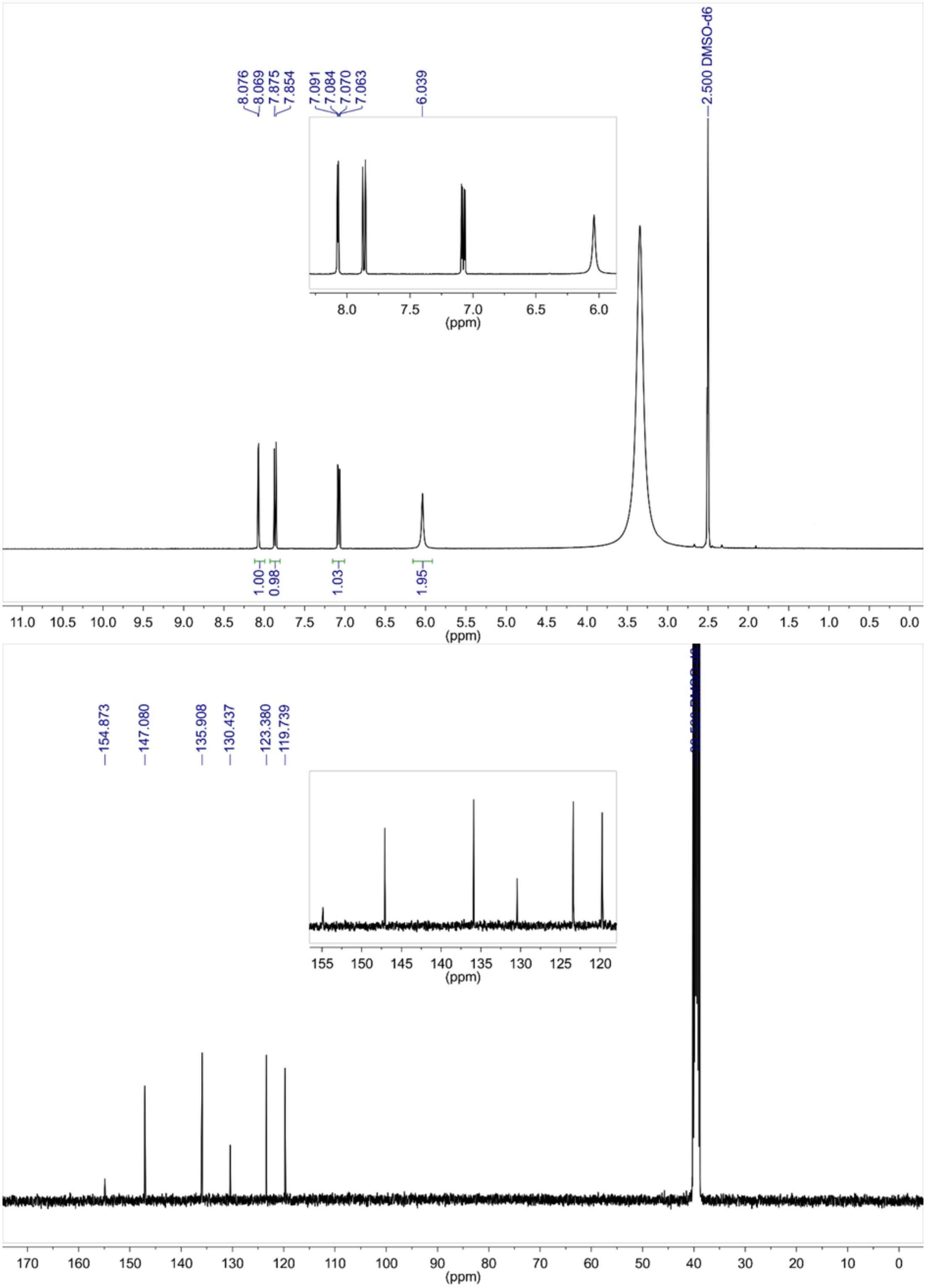


Figure S1. ^{1}H (top) and ^{13}C-NMR (bottom) spectra of $HTzPyNH_2$. DMSO-d_6.

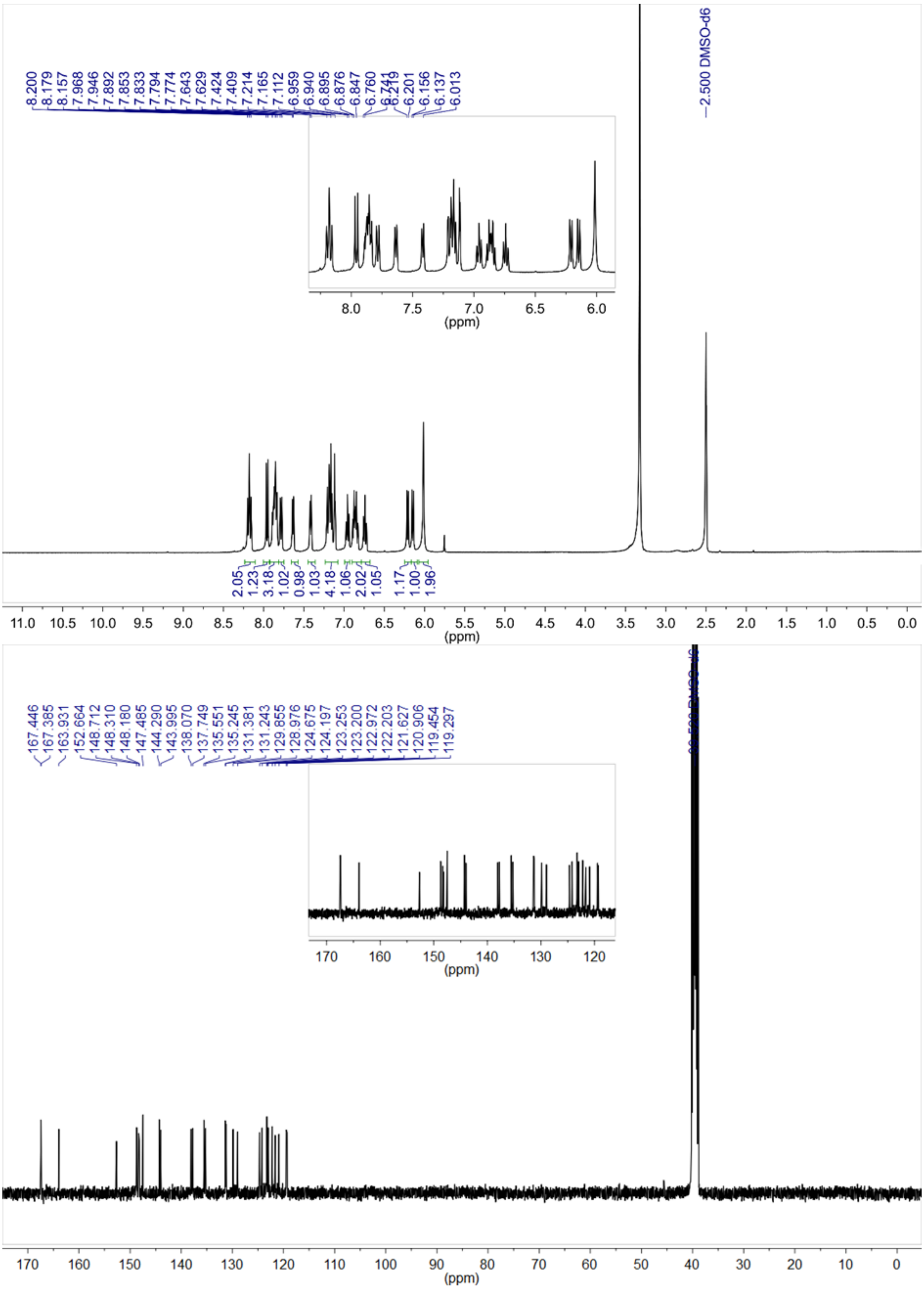


Figure S2. ^{1}H (top) and ^{13}C-NMR (bottom) spectra of $[Ir(ppy)_2(TzPyNH_2)]$. DMSO-d_6.

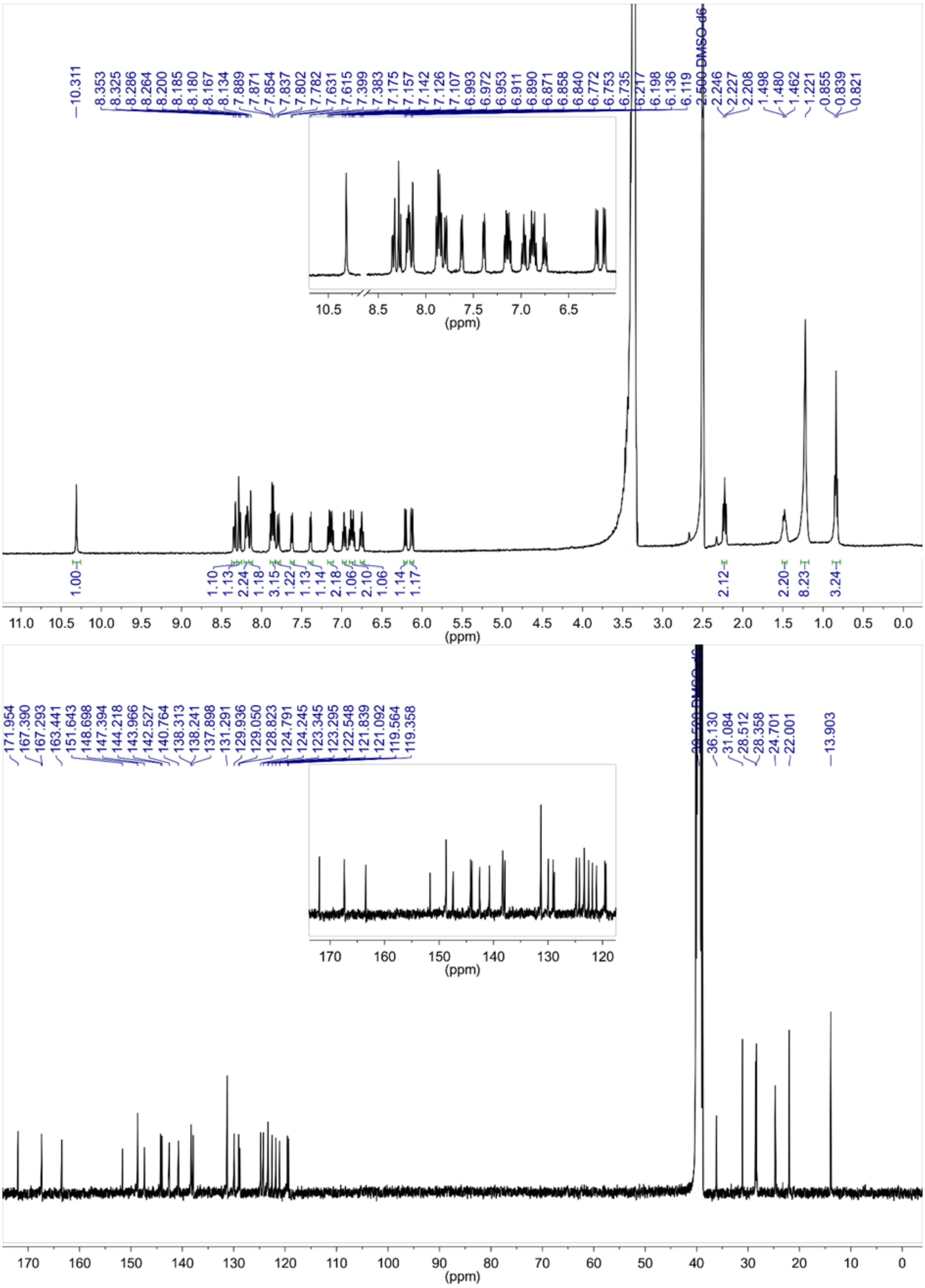
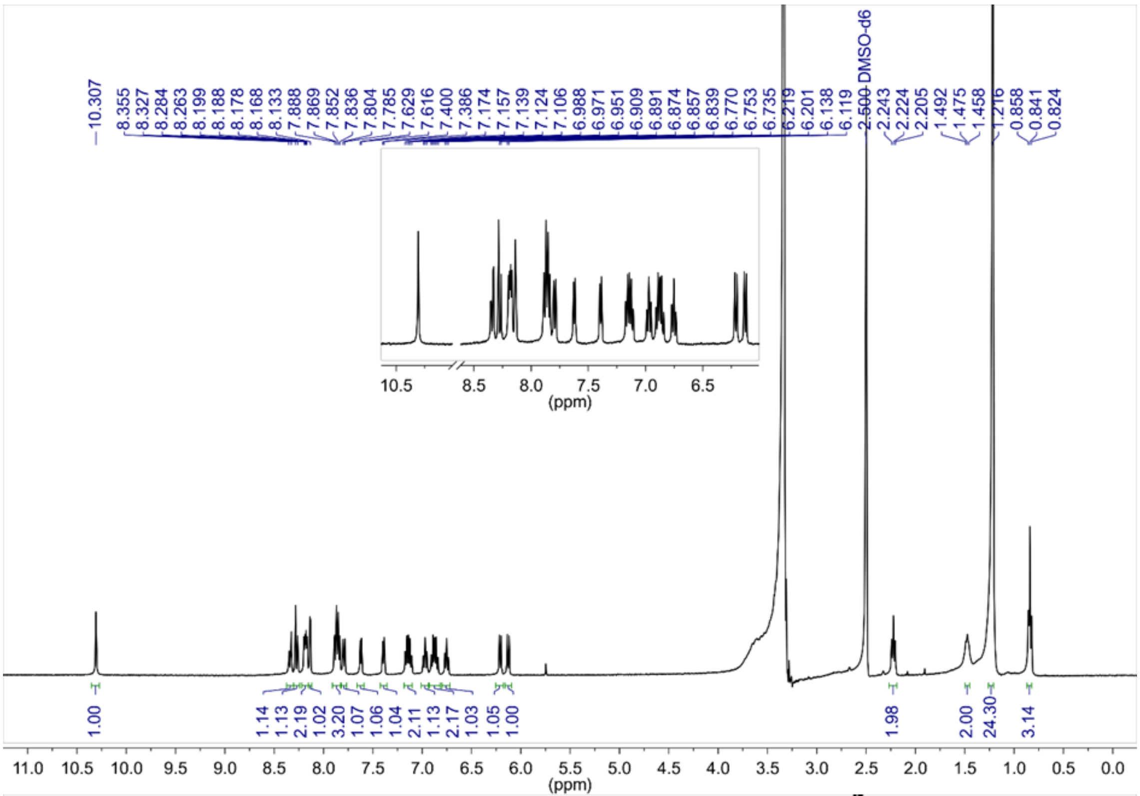


Figure S3. [1]H (top) and [13]C-NMR (bottom) spectra of [Ir(ppy)$_2$(TzPyNHC$_{8sat}$)]. DMSO-d_6.



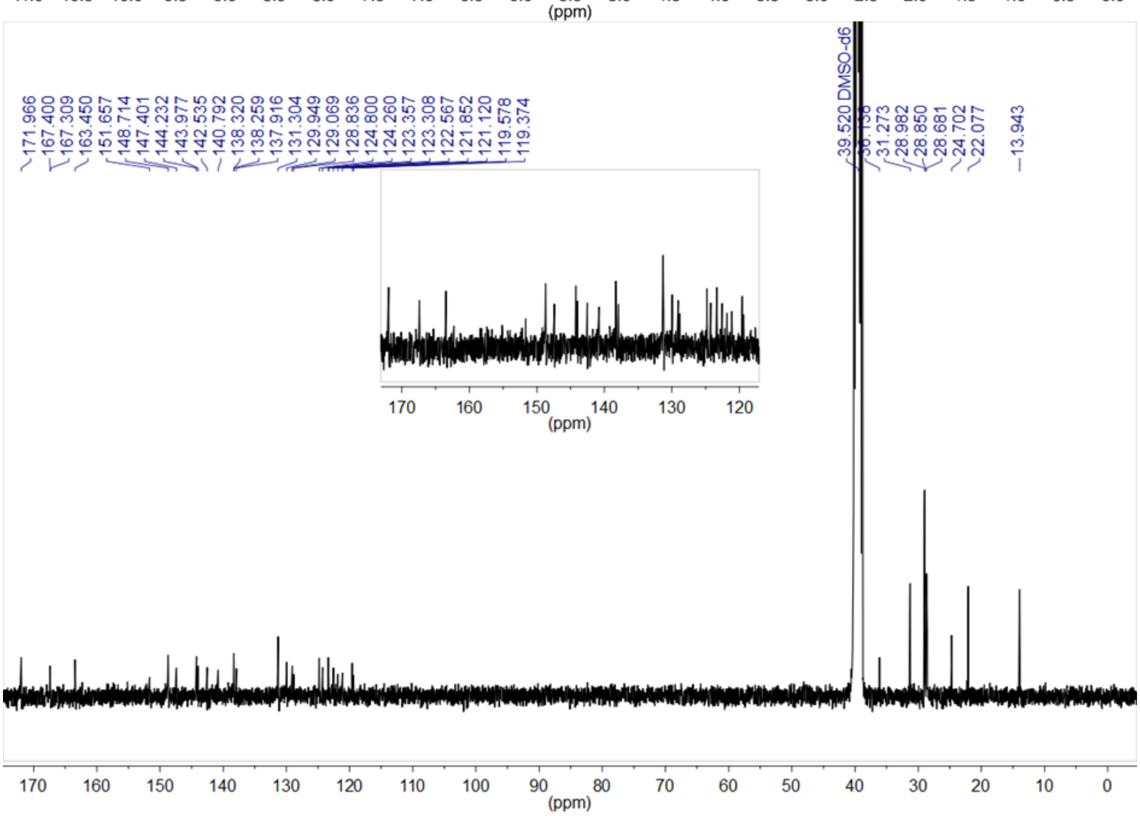
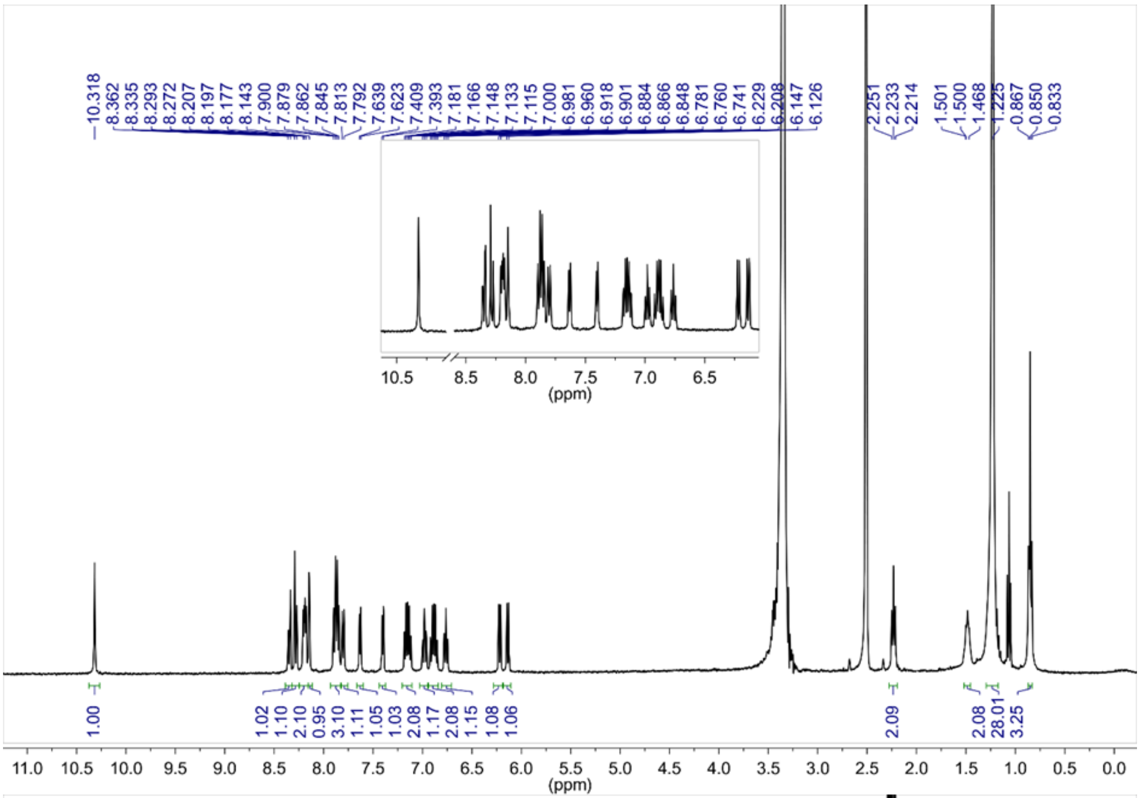


Figure S4. [1]H (top) and [13]C-NMR (bottom) spectra of [Ir(ppy)$_2$(TzPyNHC$_{16sat}$)]. DMSO-d_6.



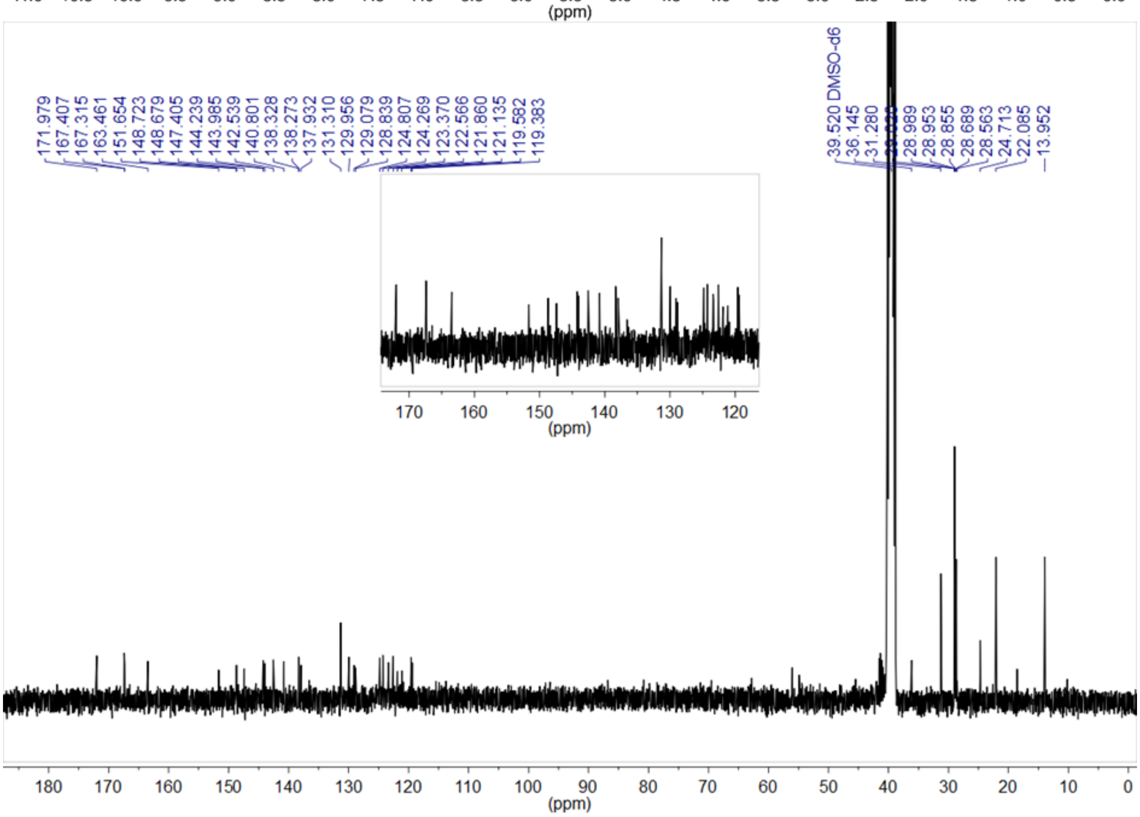


Figure S5. ^{1}H (top) and ^{13}C-NMR (bottom) spectra of [Ir(ppy)$_2$(TzPyNHC$_{18sat}$)]. DMSO-*d*$_6$.

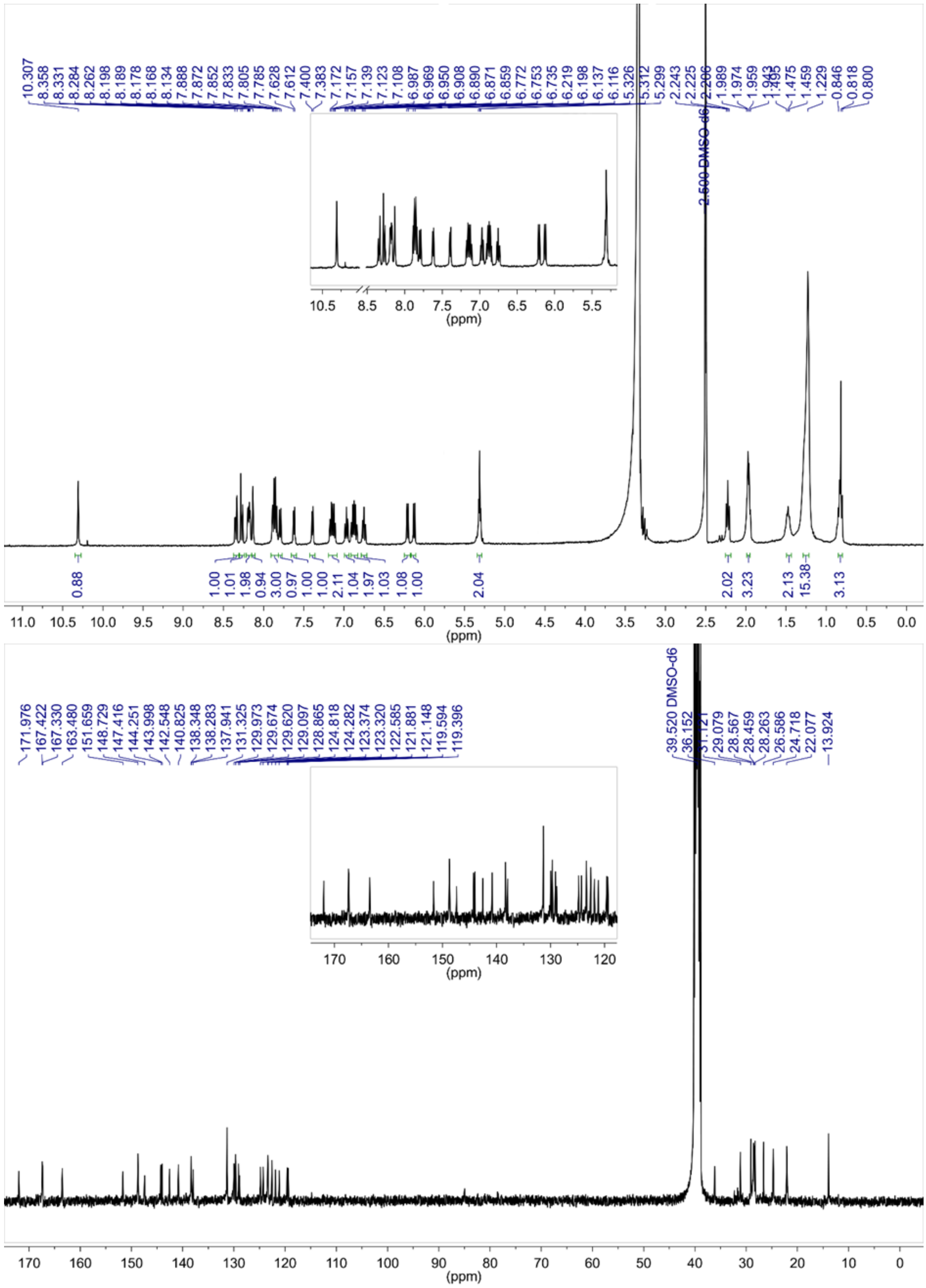


Figure S6. [1]H (top) and [13]C-NMR (bottom) spectra of [Ir(ppy)$_2$(TzPyNHC$_{16cis}$)]. DMSO-d_6.

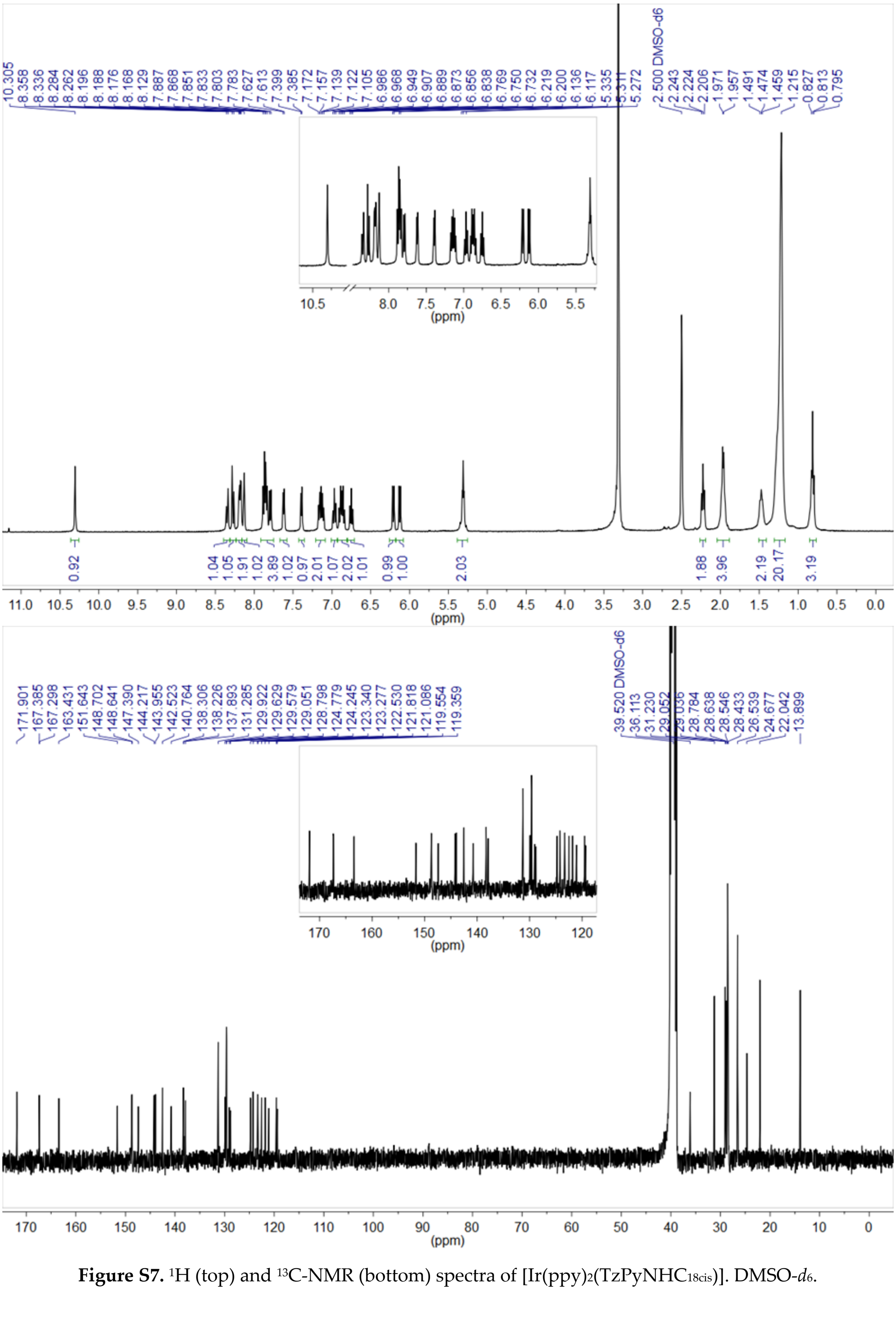


Figure S7. ^1H (top) and ^{13}C-NMR (bottom) spectra of [Ir(ppy)$_2$(TzPyNHC$_{18cis}$)]. DMSO-d_6.

All the mass spectra were recorded from solutions in methanol.

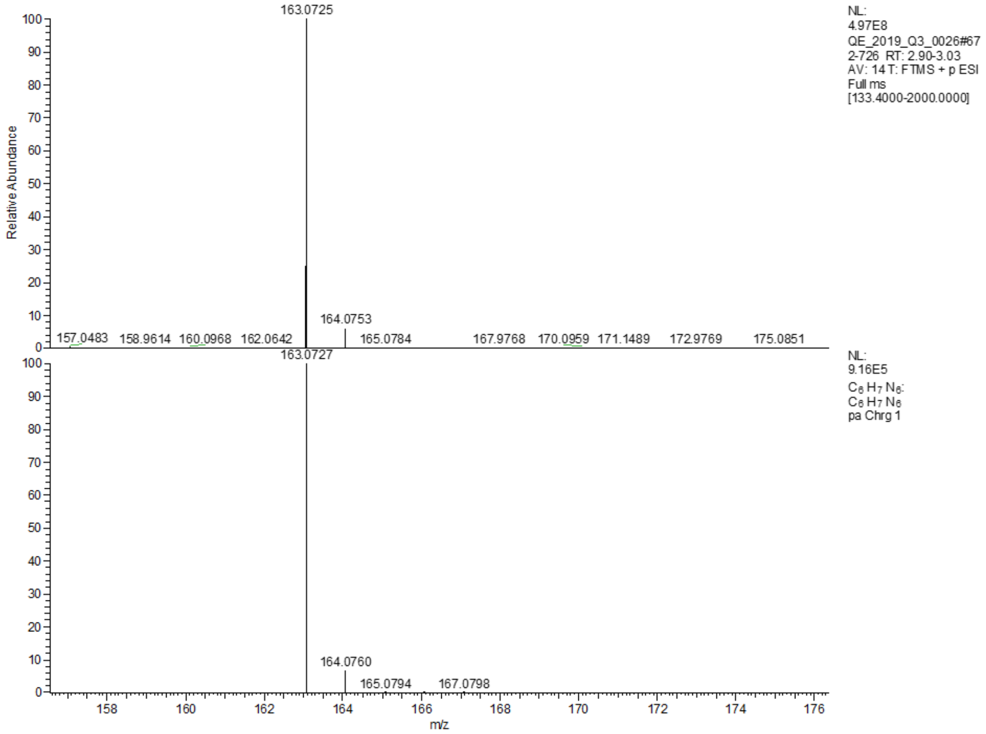


Figure S8. ESI-HRMS spectra of $HTzPyNH_2$.

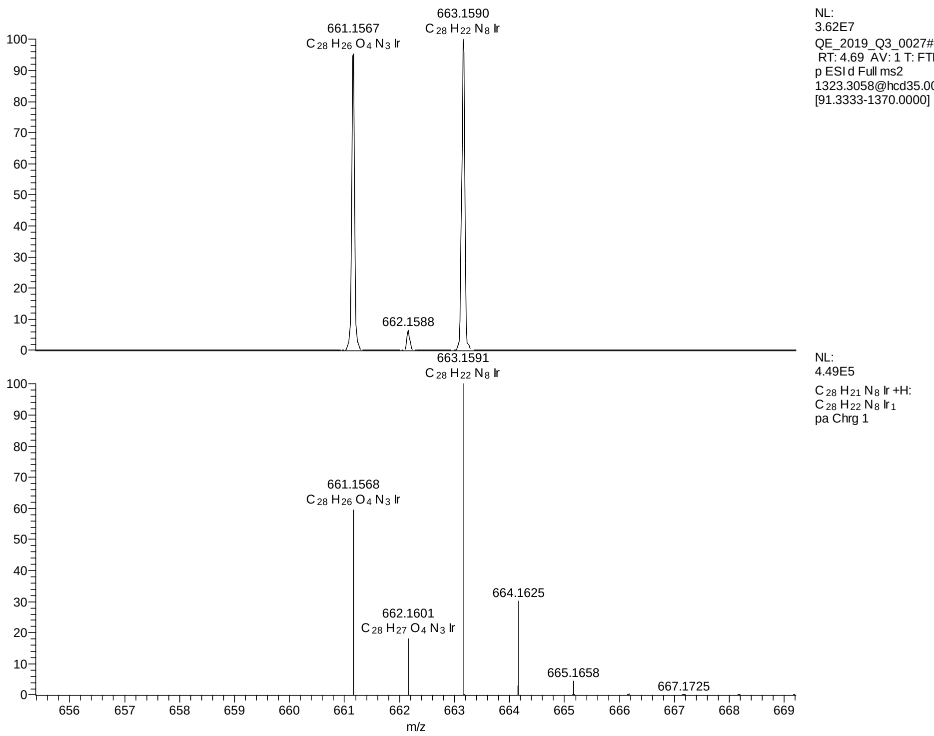


Figure S9. ESI-HRMS spectra of $[Ir(ppy)_2(TzPyNH_2)]$.

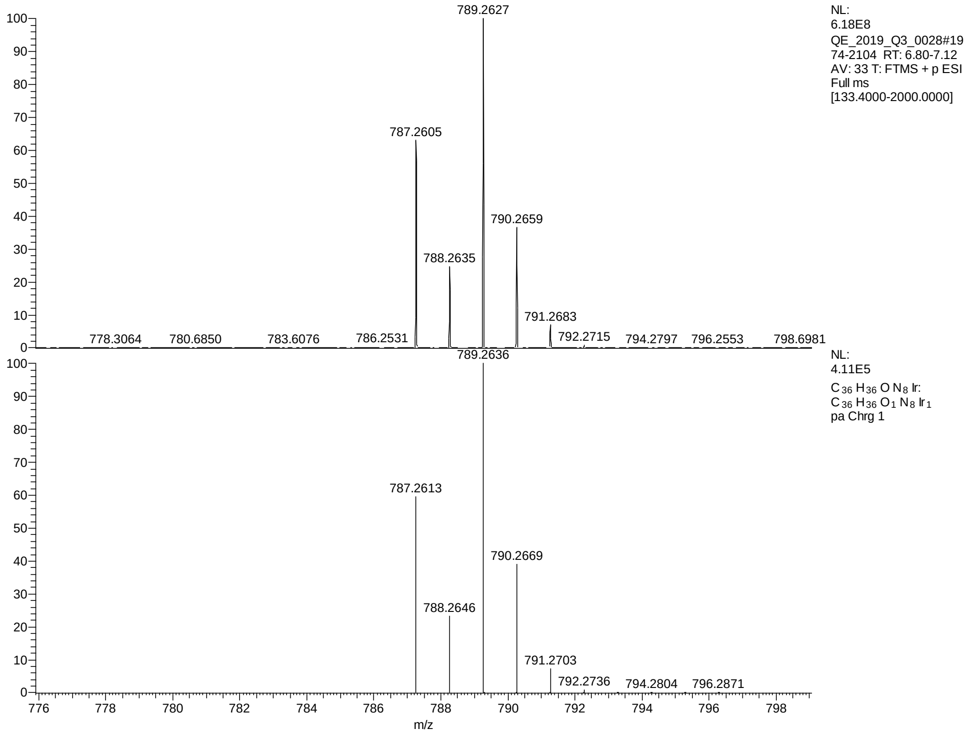


Figure S10. ESI-HRMS spectra of [Ir(ppy)$_2$(TzPyNHC$_{8sat}$)].

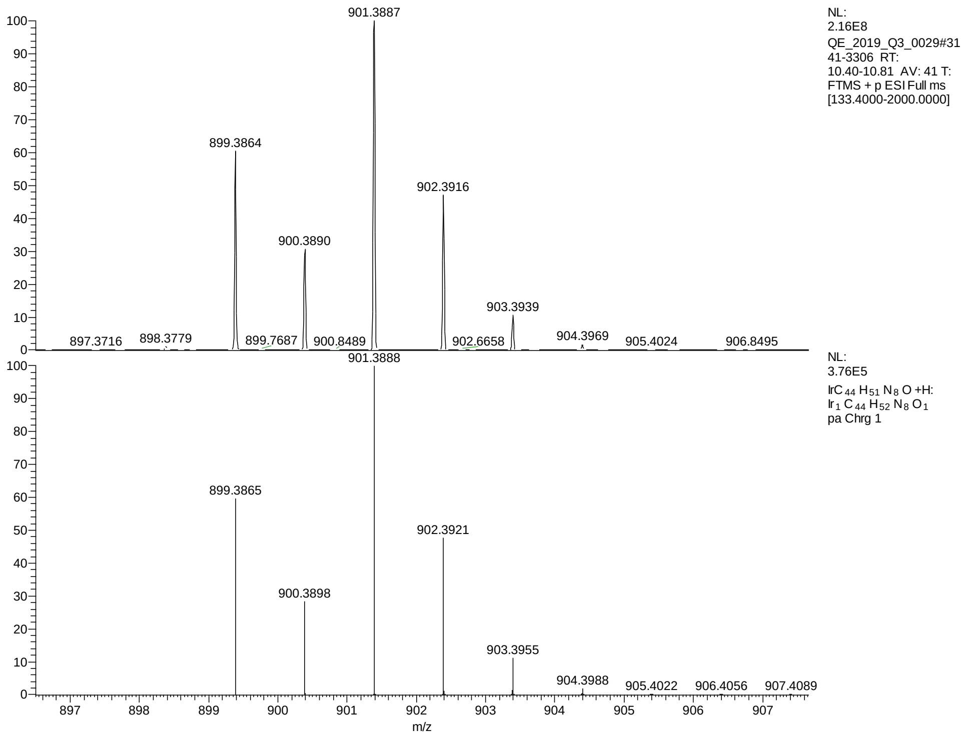


Figure S11. ESI-HRMS spectra of [Ir(ppy)$_2$(TzPyNHC$_{16sat}$)].

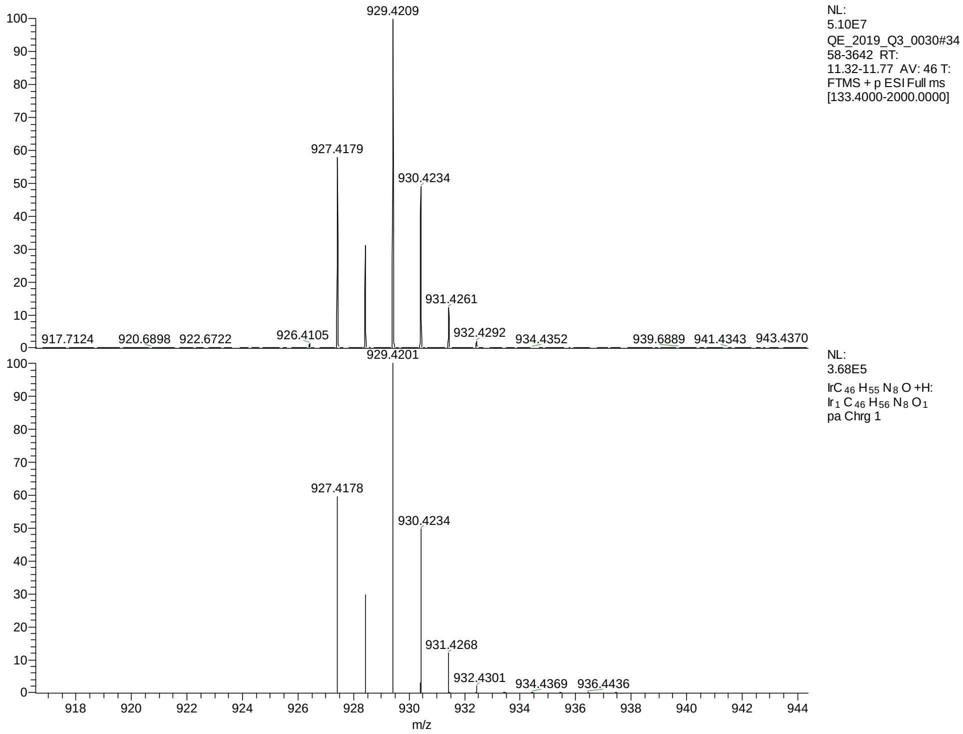


Figure S12. ESI-HRMS spectra of [Ir(ppy)2(TzPyNHC18sat)].

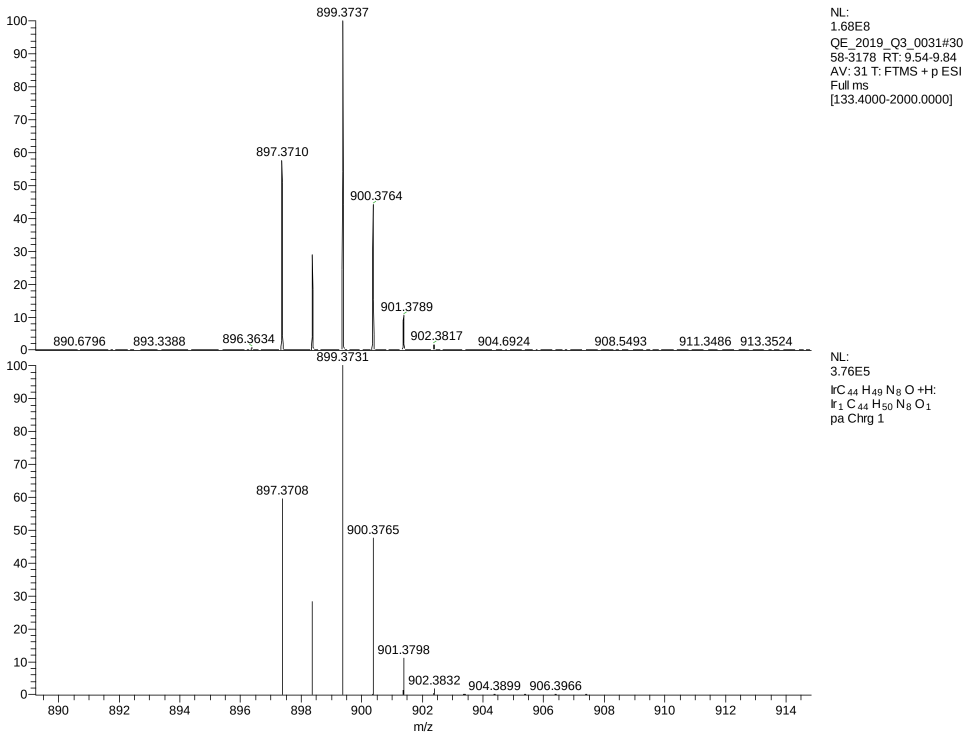


Figure S13. ESI-HRMS spectra of [Ir(ppy)2(TzPyNHC16cis)].

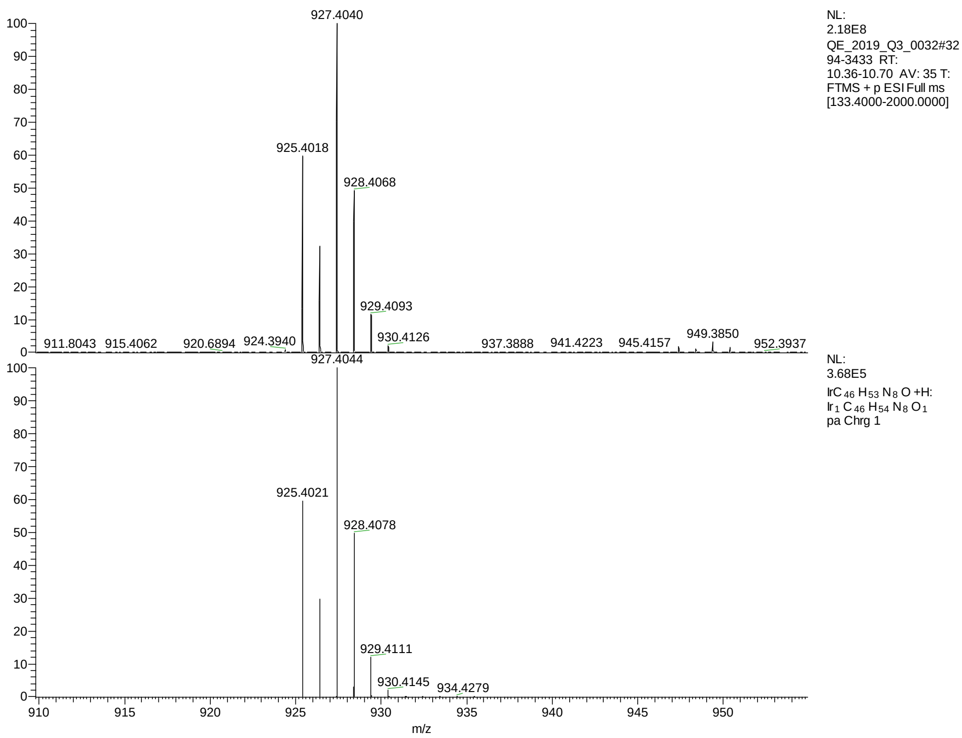


Figure S14. ESI-HRMS spectra of [Ir(ppy)$_2$(TzPyNHC$_{18cis}$)].

Table S1. Photophysical data of 10^{-5} M solution of the reported iridium complexes in aqueous and lipophilic solvents.

Complex	Solvent [a]	λ_{abs} [nm] (10^4 ε [M^{-1} cm^{-1}])	λ_{em} [nm] [b]	τ_{aer} [ns][c]	Φ_{aer} [d]
[Ir(**ppy**)$_2$ (**TzPyNH$_2$**)]	Lys. Fluid	272 (3.92), 394 (1.03), 435 (0.64)	484, 508	21 (6), 493 (94)	0.018
	PBS	272 (4.56), 349 (1.76), 429 (0.60)	484, 508	22 (6), 474 (94)	0.014
	Ethyl Laurate	276 (1.34), 372 (1.38), 445 (1.04)	484, 520, 555$_{sh}$	17 (63), 89 (37)	0.010
[Ir(**ppy**)$_2$ (**TzPyNHC$_{8sat}$**)]	Lys. Fluid	294 (0.43)	500, 530	72 (77), 422 (23)	0.042
	PBS	286 (2.71), 395 (0.87), 431 (0.62)	493, 520	52 (79), 321 (21)	0.009
	Ethyl Laurate	285 (5.90), 413 (0.76), 457 (0.35)	493, 523	48 (52), 116 (48)	0.023
[Ir(**ppy**)$_2$ (**TzPyNHC$_{16sat}$**)]	Lys. Fluid	293 (0.19)	500, 530	45 (50), 214 (50)	0.024
	PBS	289 (0.92), 391 (0.44), 433 (0.40)	495, 526	44 (45), 179 (55)	0.013
	Ethyl Laurate	285 (2.43),412 (0.95), 455 (0.73)	495, 526	78 (65), 243 (35)	0.015
[Ir(**ppy**)$_2$ (**TzPyNHC$_{18sat}$**)]	Lys. Fluid	265 (0.13)	502, 526	121 (67), 509 (33)	0.101
	PBS	281 (0.43)	498, 530	187 (63), 734 (37)	0.082
	Ethyl Laurate	284 (0.89), 416 (0.56), 455 (0.49)	498, 530	173 (70), 873 (30)	0.086
[Ir(**ppy**)$_2$ (**TzPyNHC$_{16cis}$**)]	Lys. Fluid	291 (1.30), 396 (0.63), 433 (0.48)	496, 548	51 (66), 466 (34)	0.013
	PBS	284 (2.57), 395 (0.90), 428 (0.67)	496, 548	59 (55), 462 (45)	0.014
	Ethyl Laurate	277 (2.71), 392 (0.27), 460 (0.17)	489, 521	96	0.059
[Ir(**ppy**)$_2$ (**TzPyNHC$_{18cis}$**)]	Lys. Fluid	287 (1.19), 395 (0.58), 436 (0.43)	493, 537	36 (68), 249 (32)	0.015
	PBS	285 (2.67), 394 (0.88), 433 (0.60)	493, 520	58 (79), 321 (21)	0.011
	Ethyl Laurate	278 (3.73), 395 (0.45), 436 (0.27)	493, 523	48 (52), 116 (48)	0.049

[a] Aqueous solvents contain 2% DMSO. [b] "Sh" decribes a shoulder. [c] For the biexponential excited state lifetime (τ), the relative weights of the exponential curves are reported in parentheses. [d] Measured versus [Ru(**bpy**)$_3$]Cl_2 in H_2O (Φ_r = 0.028) [1].

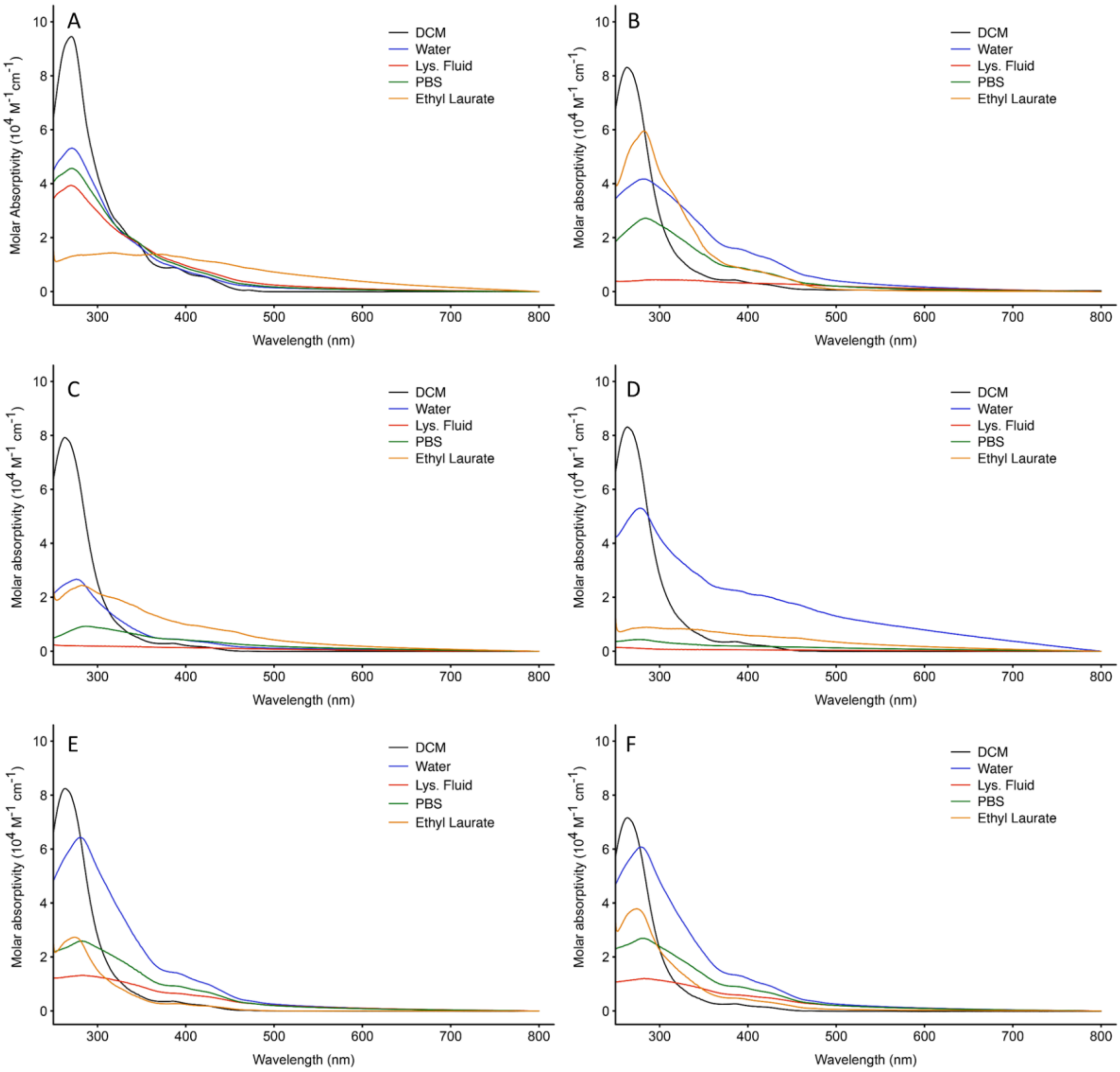


Figure S15. Absorption profiles of the reported iridium complexes from various 10^{-5} M solutions. (**A**) $[Ir(ppy)_2(TzPyNH_2)]$; (**B**) $[Ir(ppy)_2(TzPyNHC_{8sat})]$; (**C**) $[Ir(ppy)_2(TzPyNHC_{16sat})]$; (**D**) $[Ir(ppy)_2(TzPyNHC_{18sat})]$; (**E**) $[Ir(ppy)_2(TzPyNHC_{16cis})]$; (**F**) $[Ir(ppy)_2(TzPyNHC_{18cis})]$.

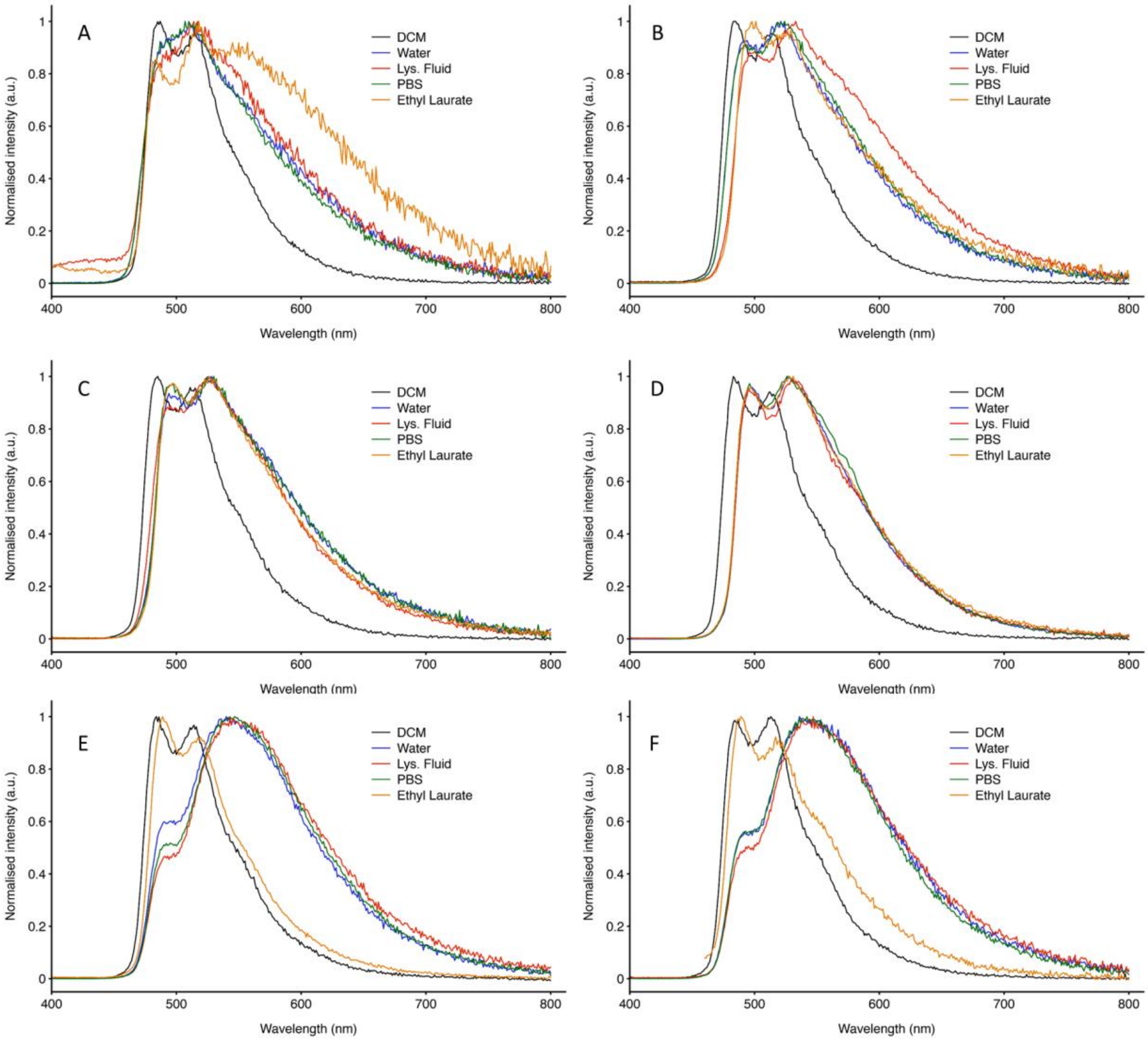


Figure S16. Emission profiles of the reported iridium complexes from various 10^{-5} M solutions. (**A**) $[Ir(ppy)_2(TzPyNH_2)]$; (**B**) $[Ir(ppy)_2(TzPyNHC_{8sat})]$; (**C**) $[Ir(ppy)_2(TzPyNHC_{16sat})]$; (**D**) $[Ir(ppy)_2(TzPyNHC_{18sat})]$; (**E**) $[Ir(ppy)_2(TzPyNHC_{16cis})]$; (**F**) $[Ir(ppy)_2(TzPyNHC_{18cis})]$.

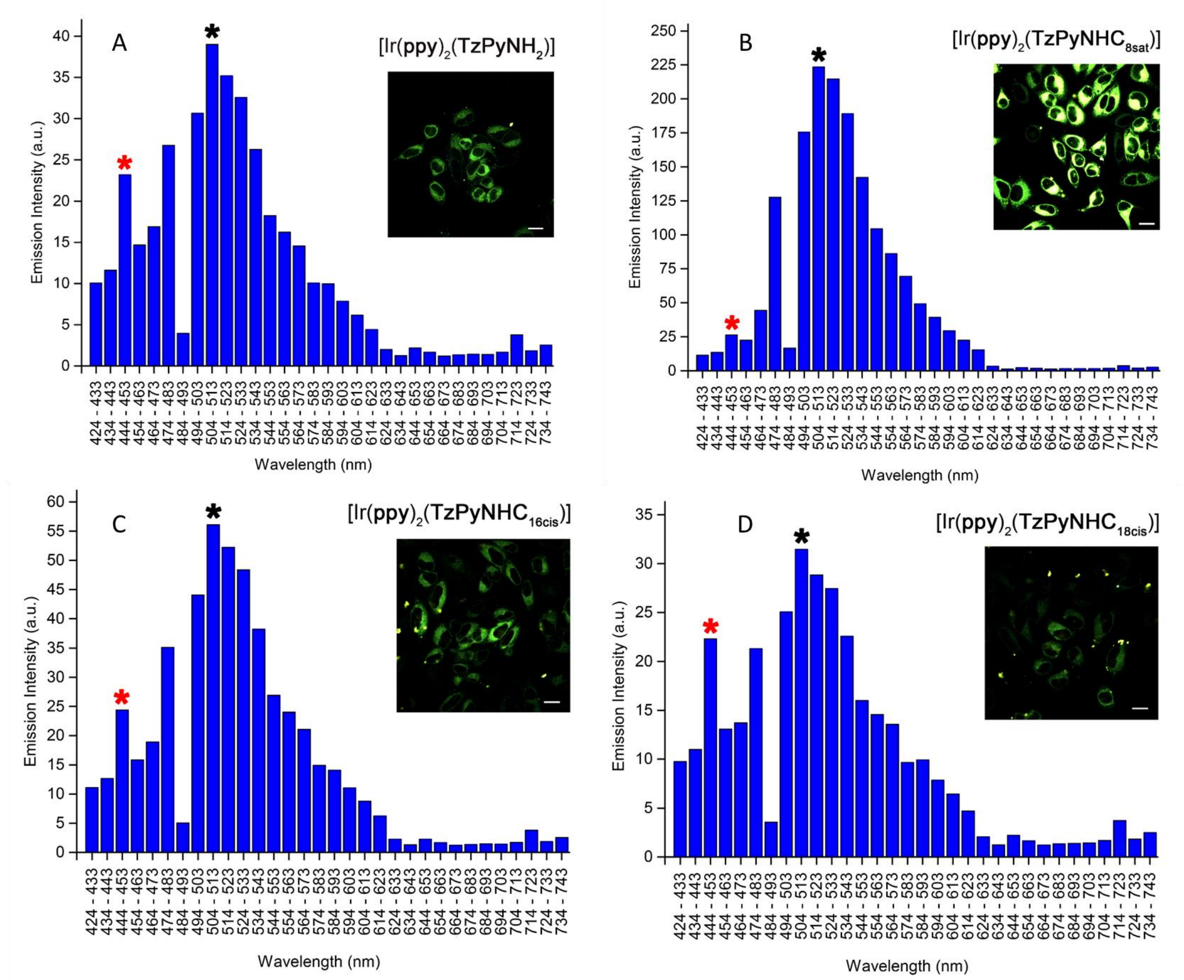


Figure S17. Emission profiles for the iridium complexes incubated in live cells. The maximum emission (black star) and the emission from endogenous species (red star) are highlighted. Scale bar = 20 μm.

References

1 K. Nakamaru, *Bull. Chem. Soc. Jpn.*, 1982, *55*, 2697–2705.