Supplementary Materials

Synthesis and characterization of Zn-salophen complexes with different D-A distances: An Approach to Tuning the Intersystem-Crossing Process

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Ⅰ. Characterization of Zn-1-4 series compounds

1. Zn-1 and intermediate product

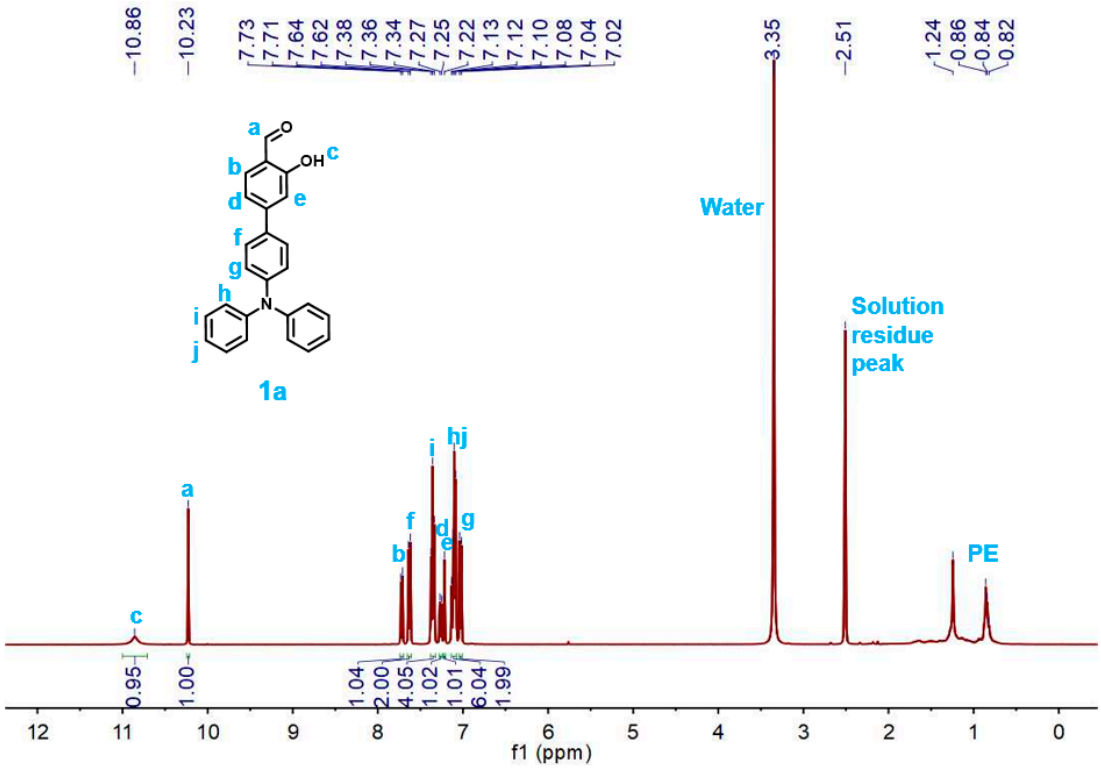


Figure S1. ^{1}H NMR of 1a (400 MHz, DMSO-d_6)

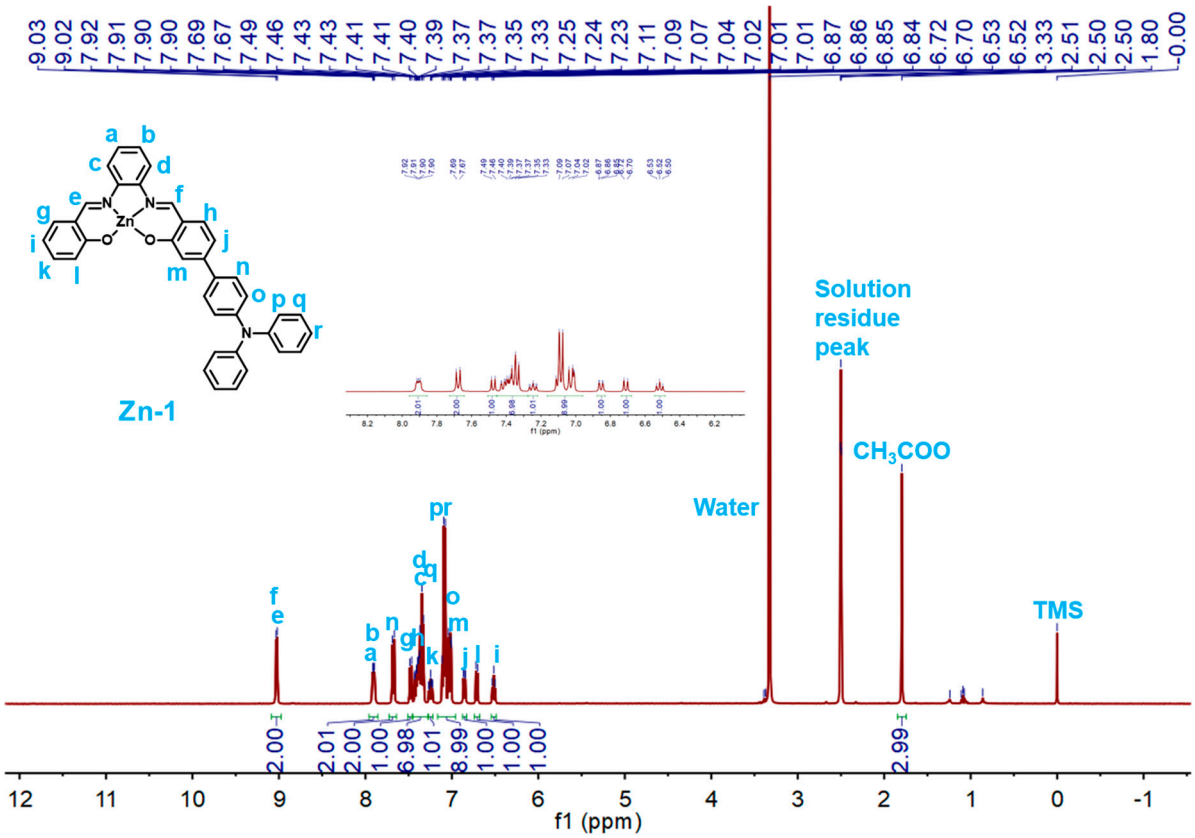


Figure S2. ^{1}H NMR of Zn-1 (400 MHz, DMSO-d$_6$)

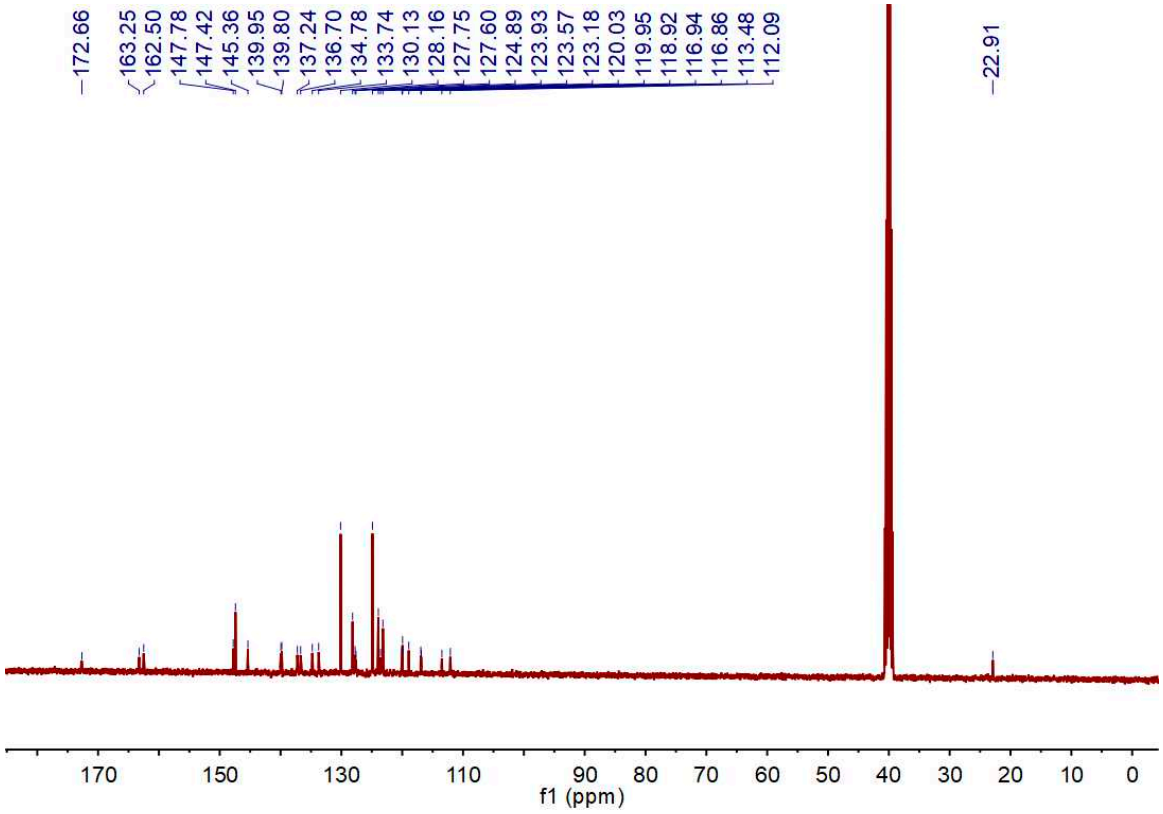


Figure S3. ^{13}C NMR of Zn-1 (400 MHz, DMSO-d$_6$)

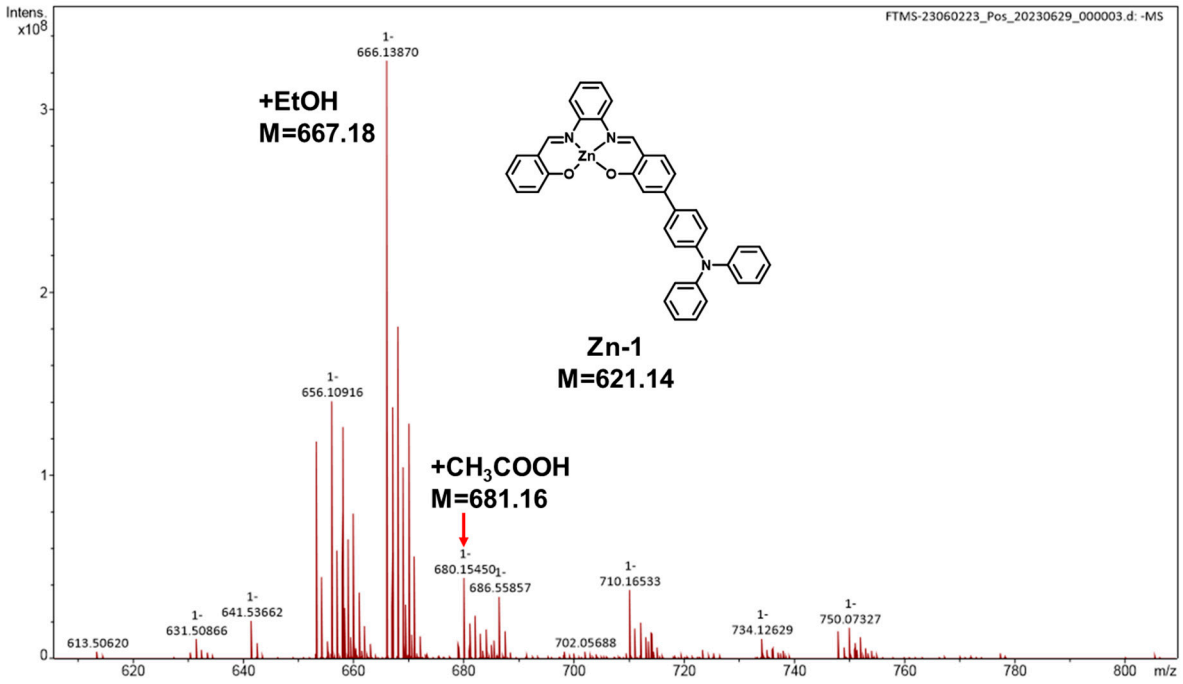


Figure S4. MS of Zn-1

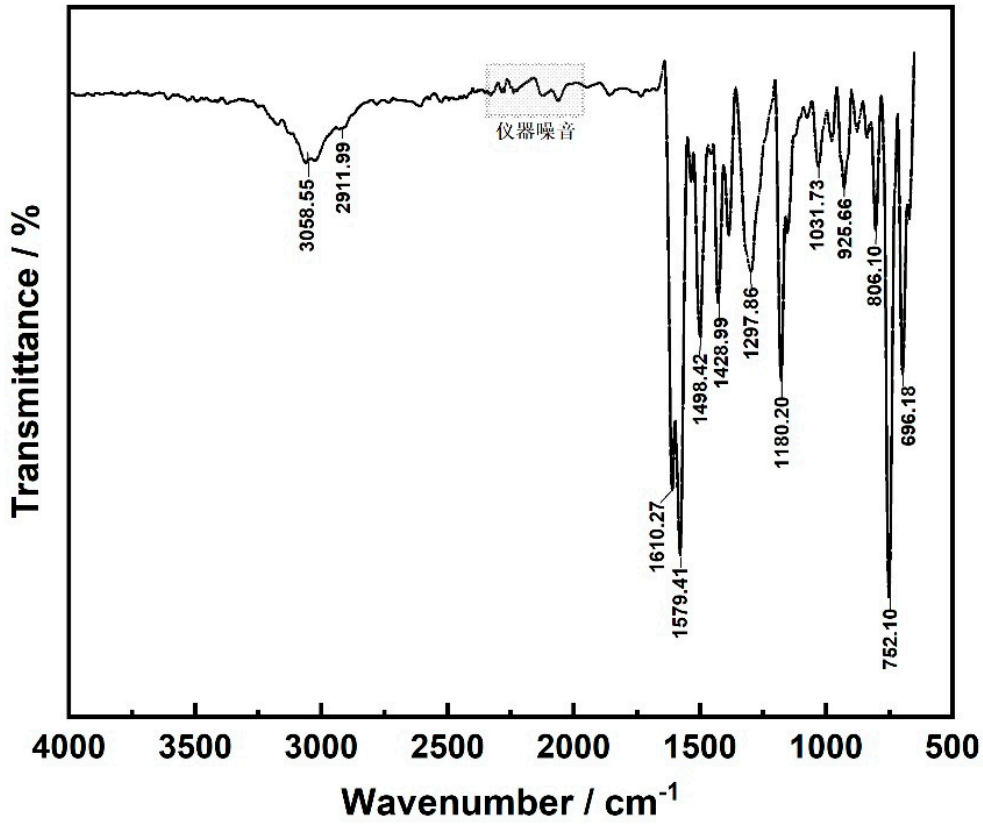


Figure S5. IR of Zn-1

2. Zn-2 and intermediate product

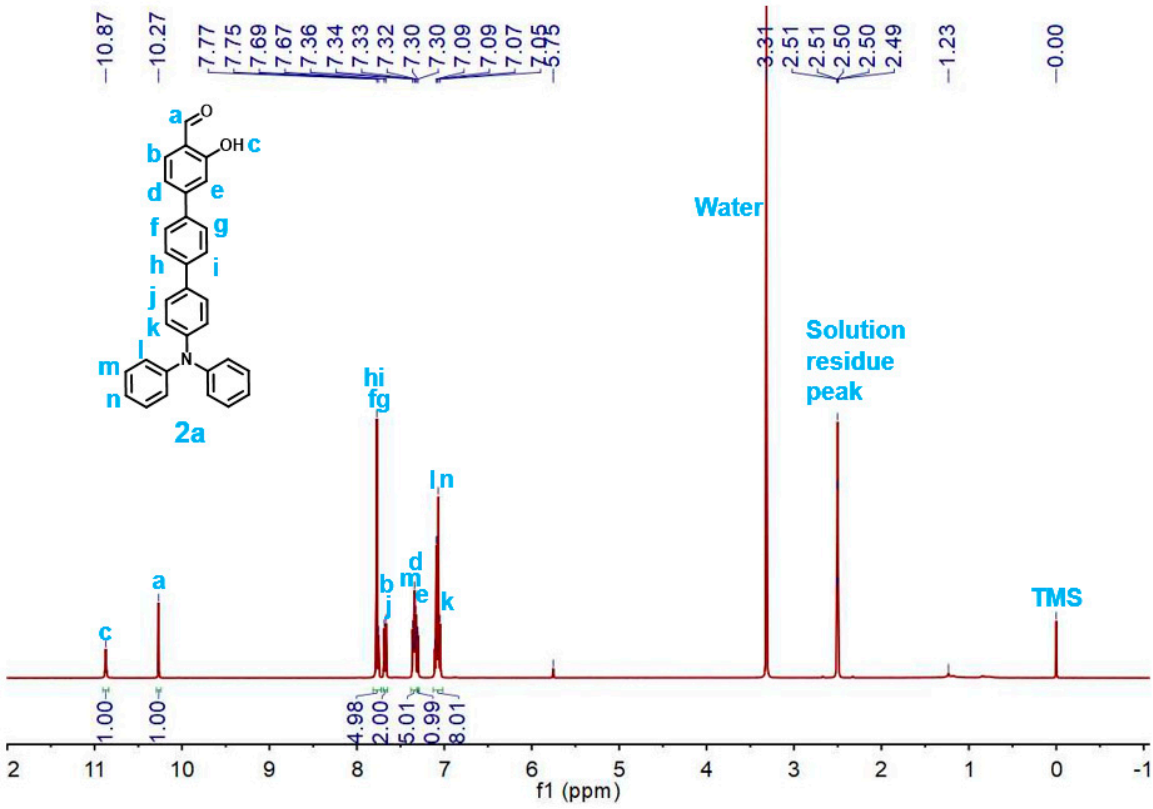


Figure S6. ^{1}H NMR of 2a (400 MHz, DMSO-d_6)

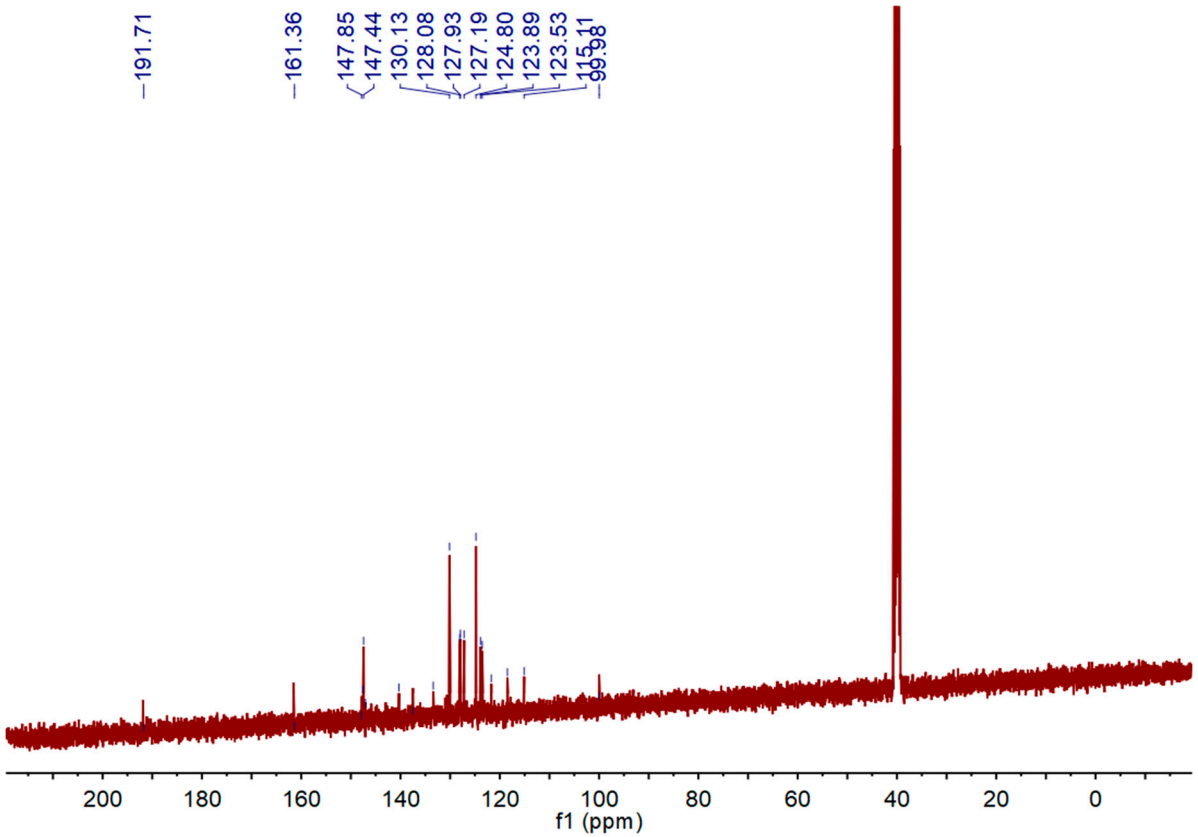
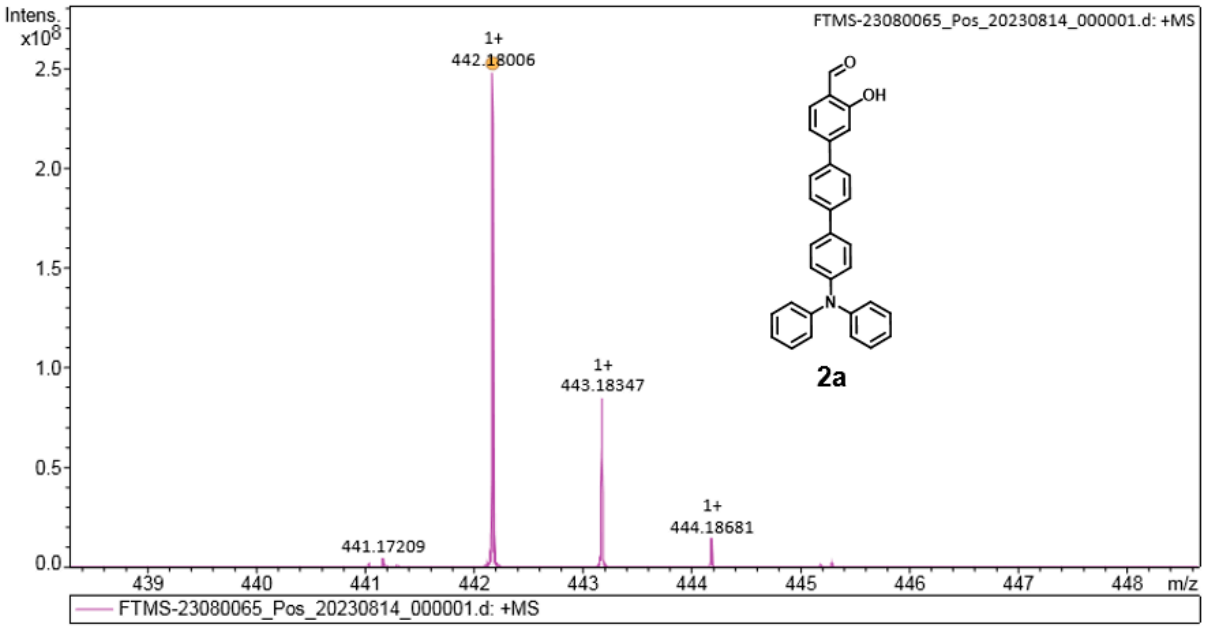


Figure S7. ^{13}C NMR of 2a (400 MHz, DMSO-d_6)



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	Mean err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
442.180056	1	C31H24NO2	100.00	442.180155	0.2	0.2	1.9	21.0	even	ok

Figure S8. MS of 2a

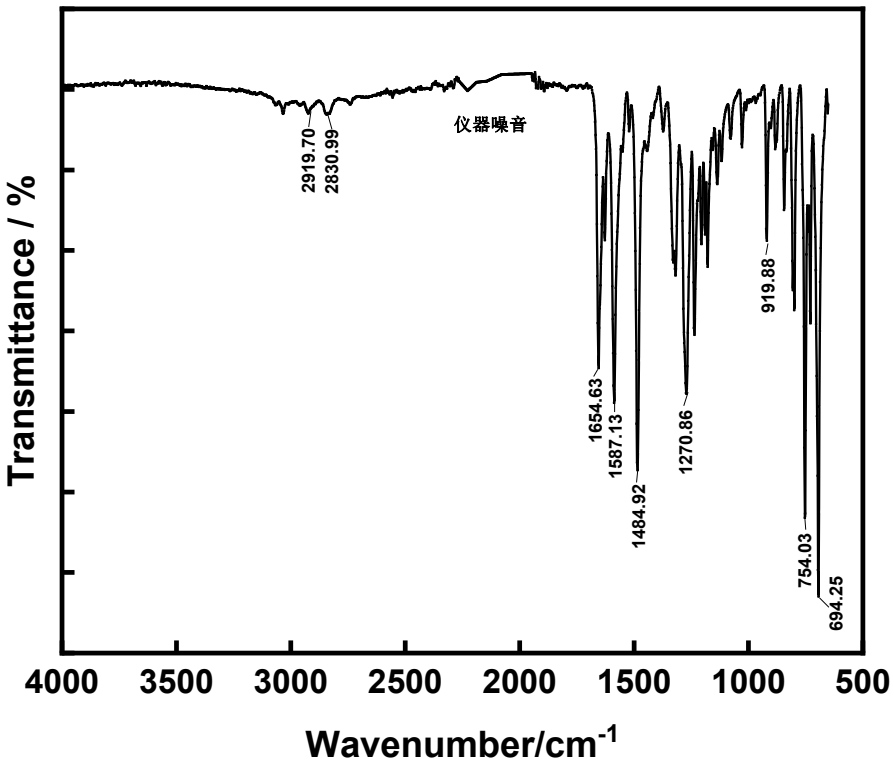


Figure S9. IR of 2a

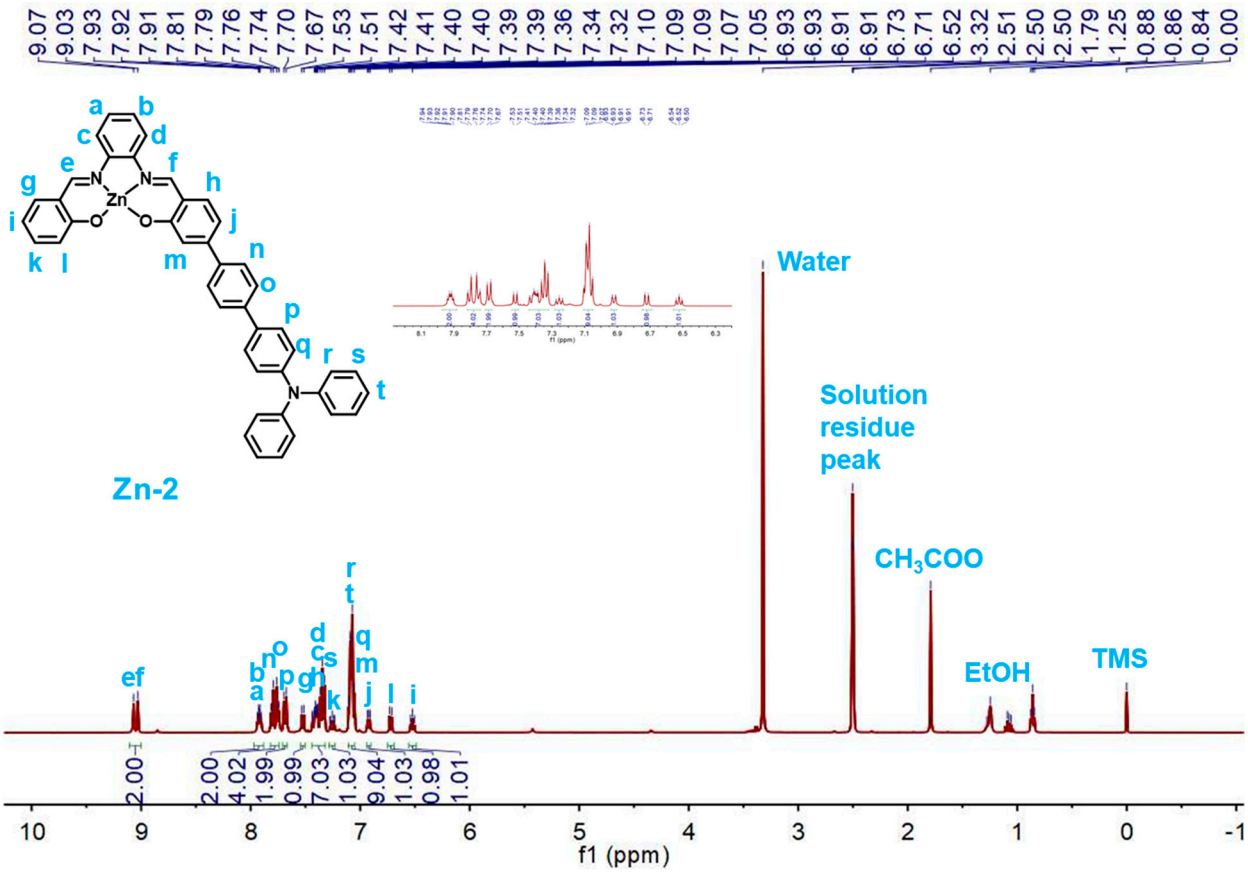


Figure S10. ^{1}H NMR of Zn-2 (400 MHz, DMSO-d$_6$)

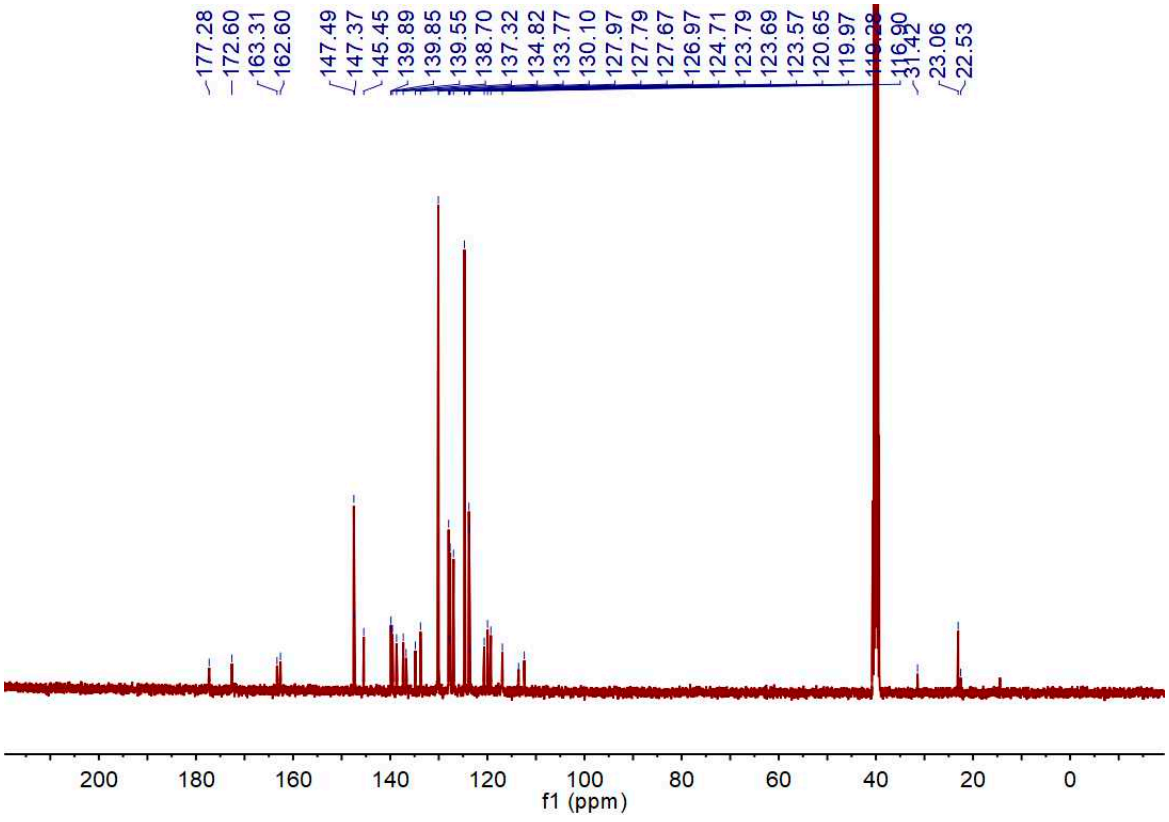


Figure S11. ^{13}C NMR of Zn-2 (400 MHz, DMSO-d$_6$)

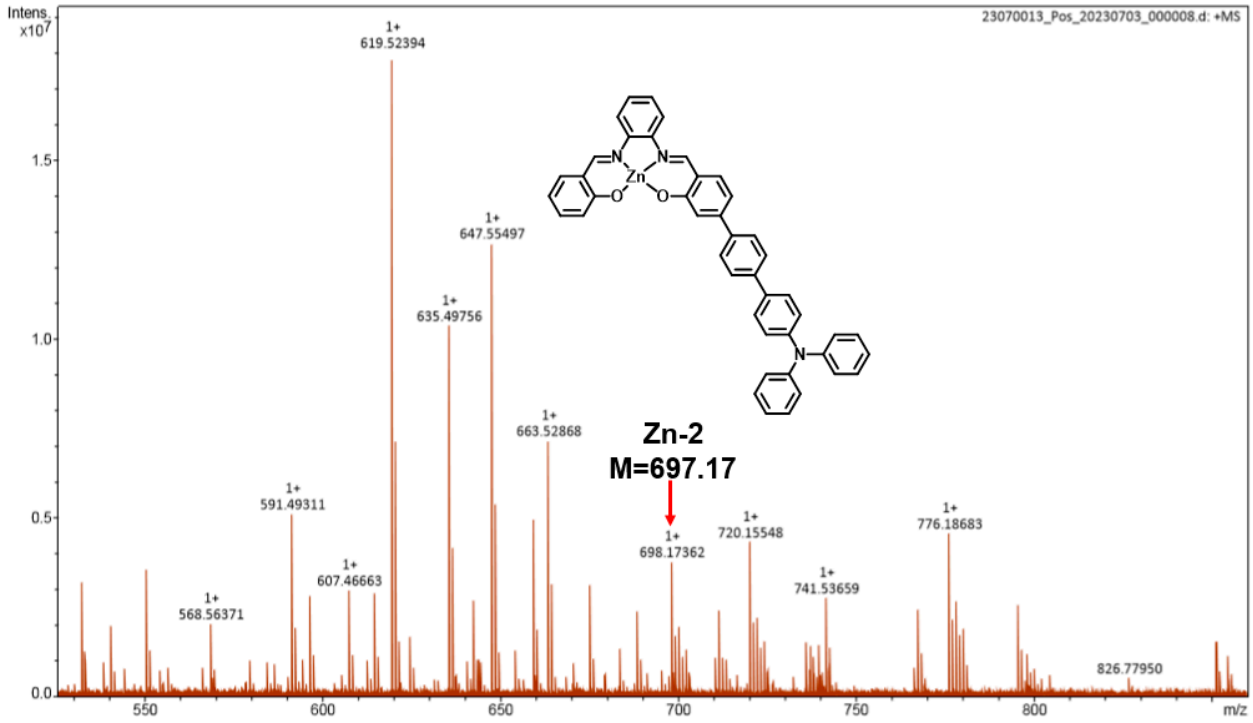


Figure S12. MS of Zn-2

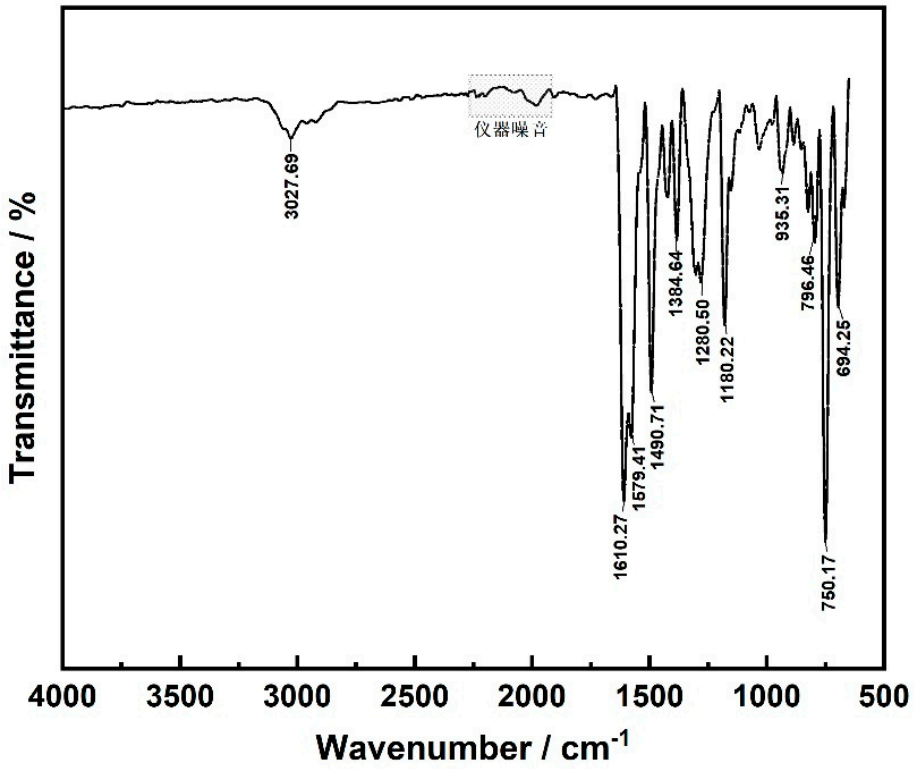


Figure S13. IR of Zn-2

3. Zn-3 and intermediate product

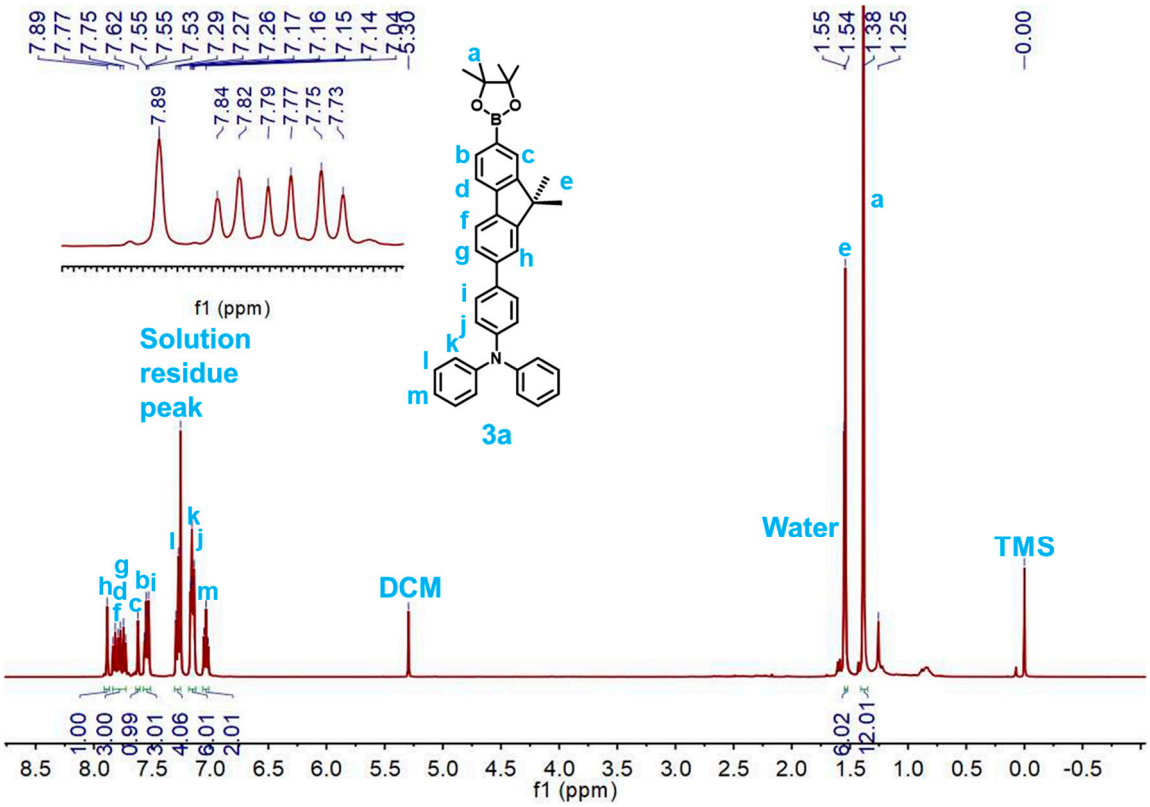


Figure S14. ^{1}H NMR of 3a (400 MHz, $CDCl_3$)

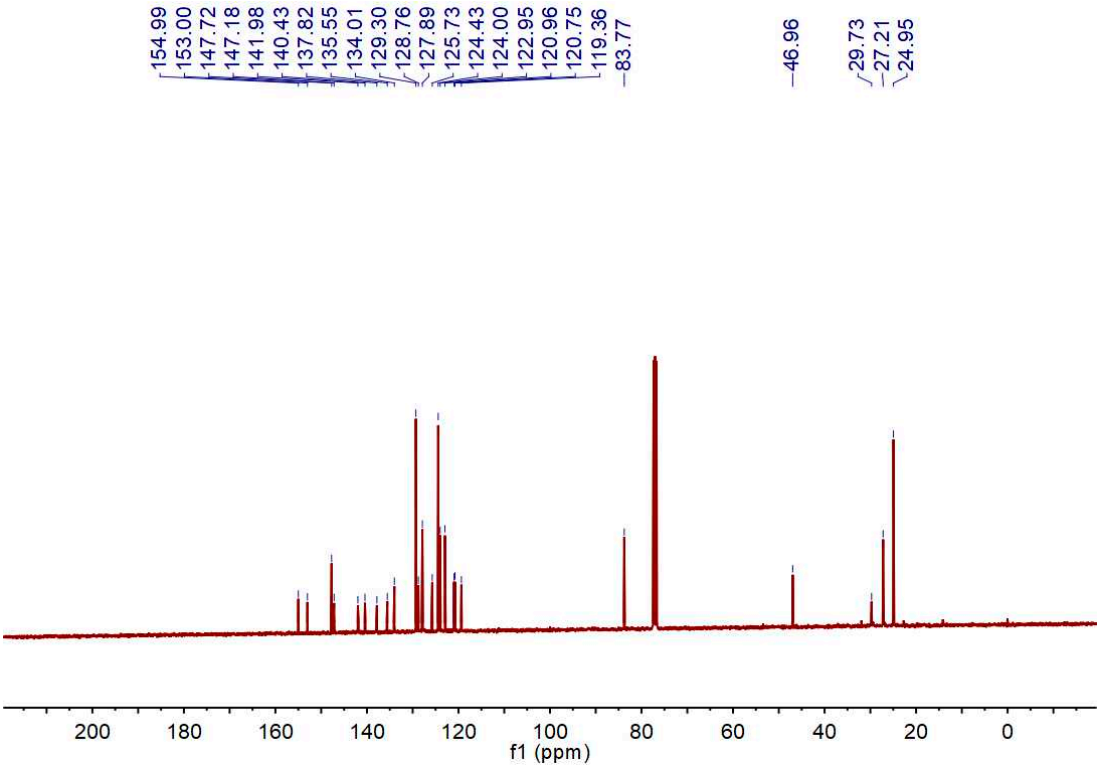


Figure S15. ^{13}C NMR of 3a (400 MHz, $CDCl_3$)

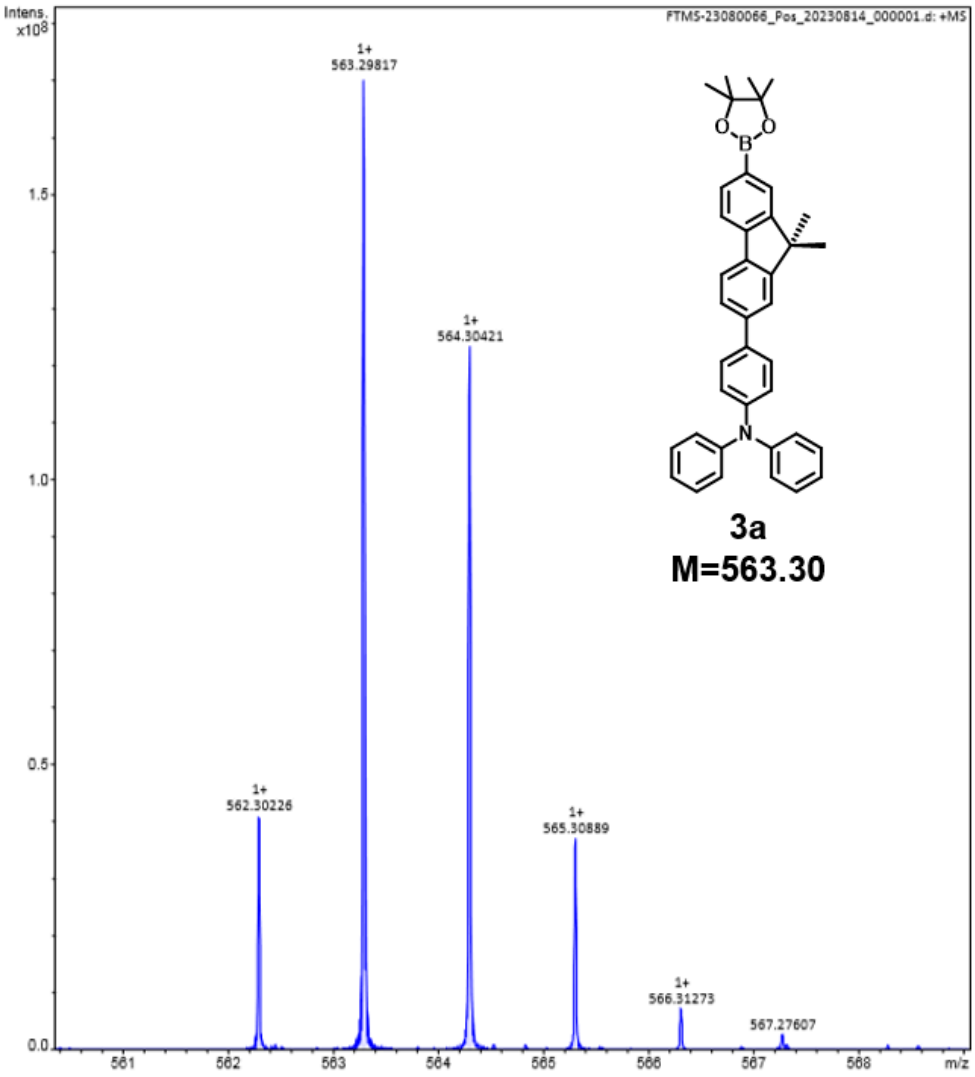


Figure S16. MS of 3a

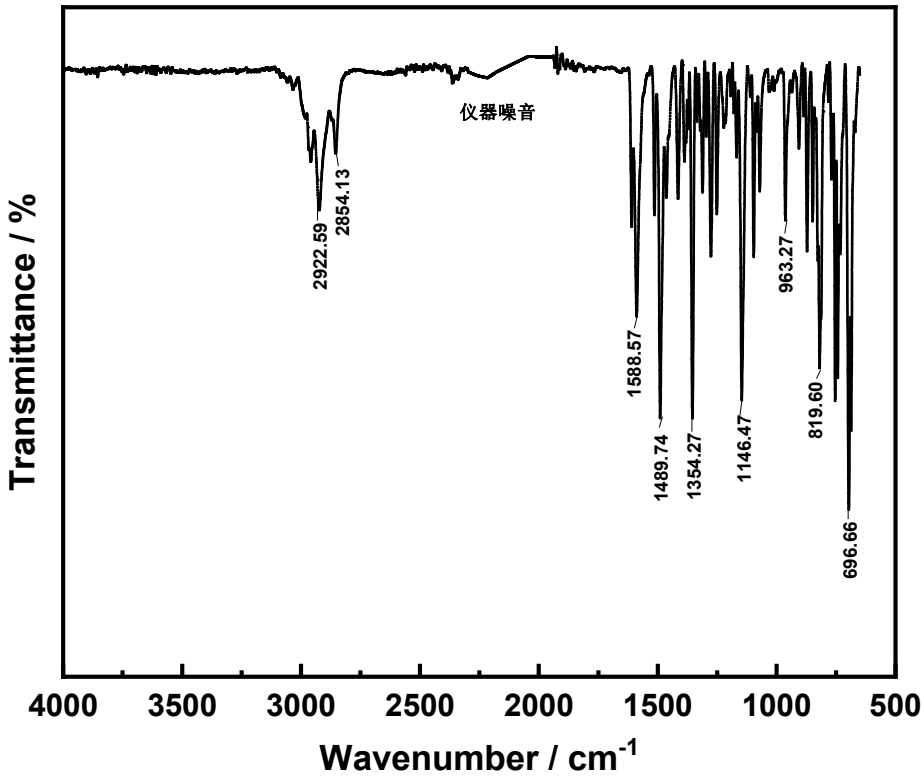


Figure S17. IR of 3a

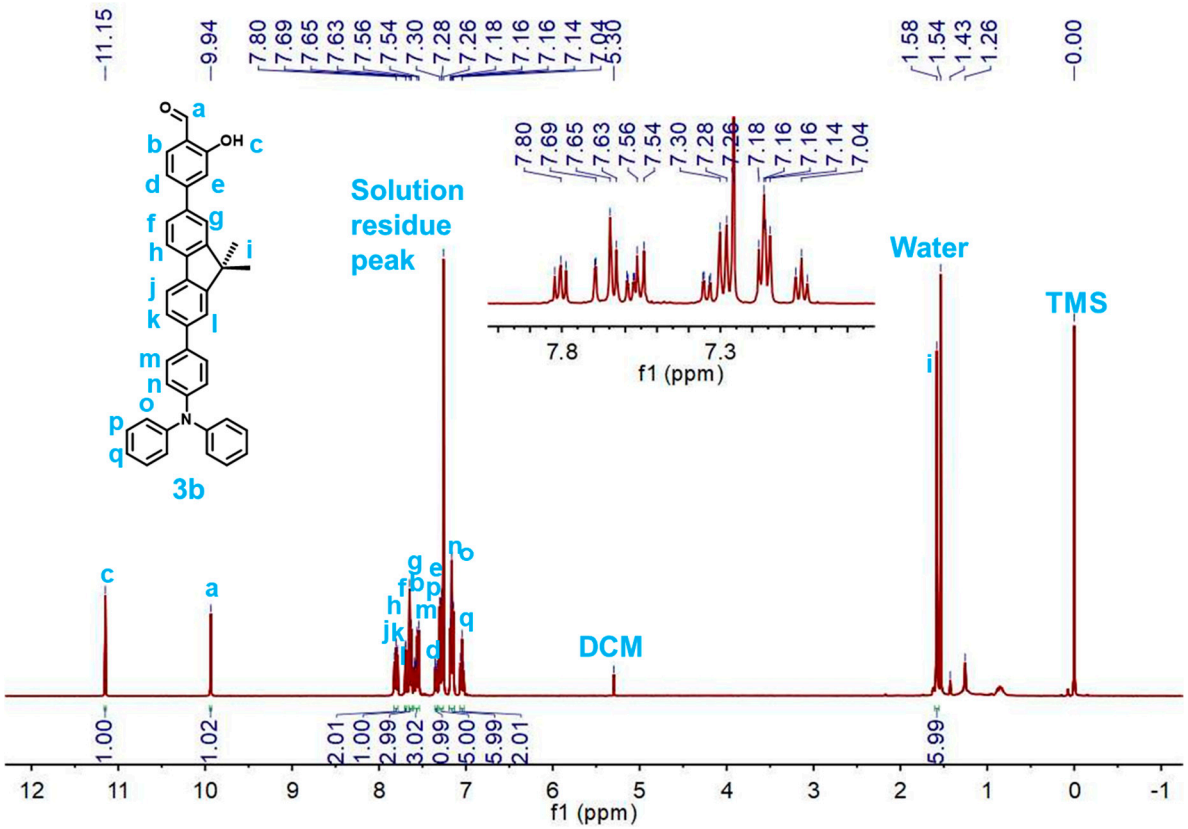


Figure S18. ^{1}H NMR of 3b (400 MHz, $CDCl_3$)

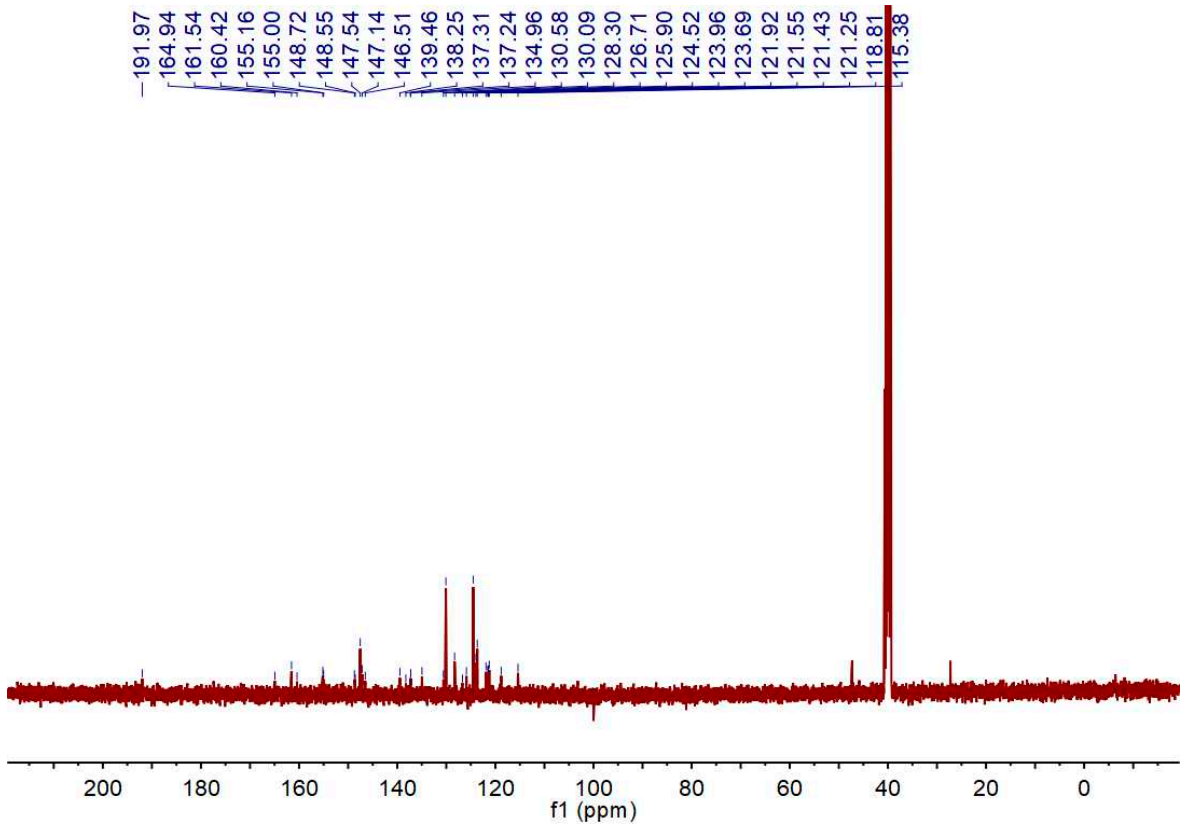


Figure S19. ^{13}C NMR of 3b (400 MHz, DMSO-d_6)

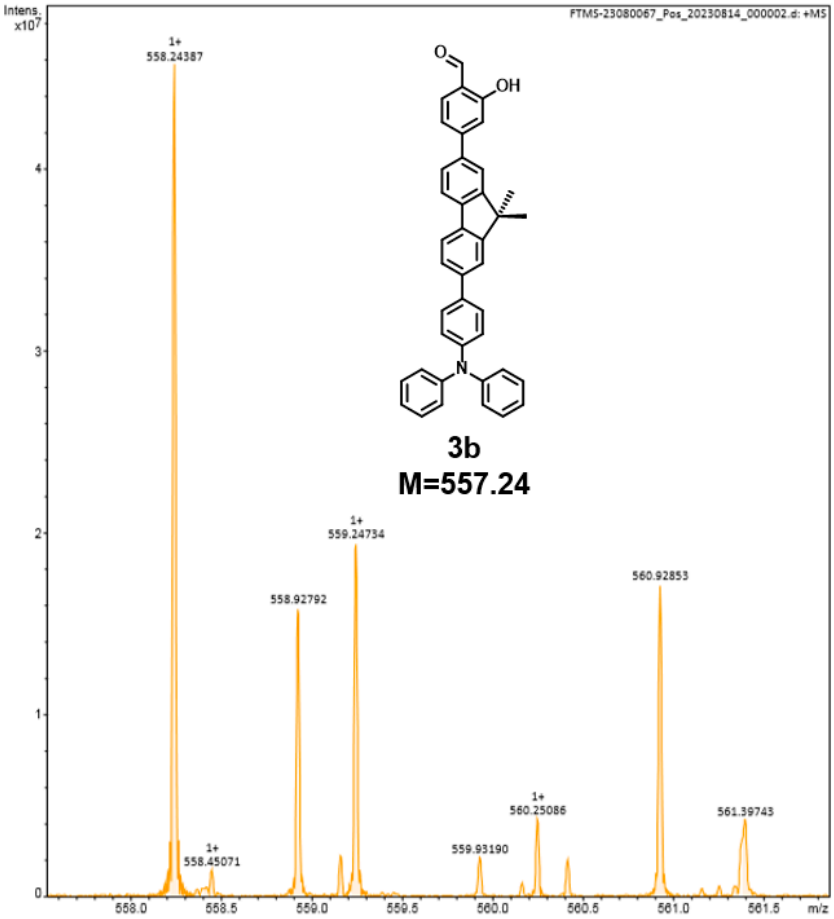


Figure S20. MS of 3b

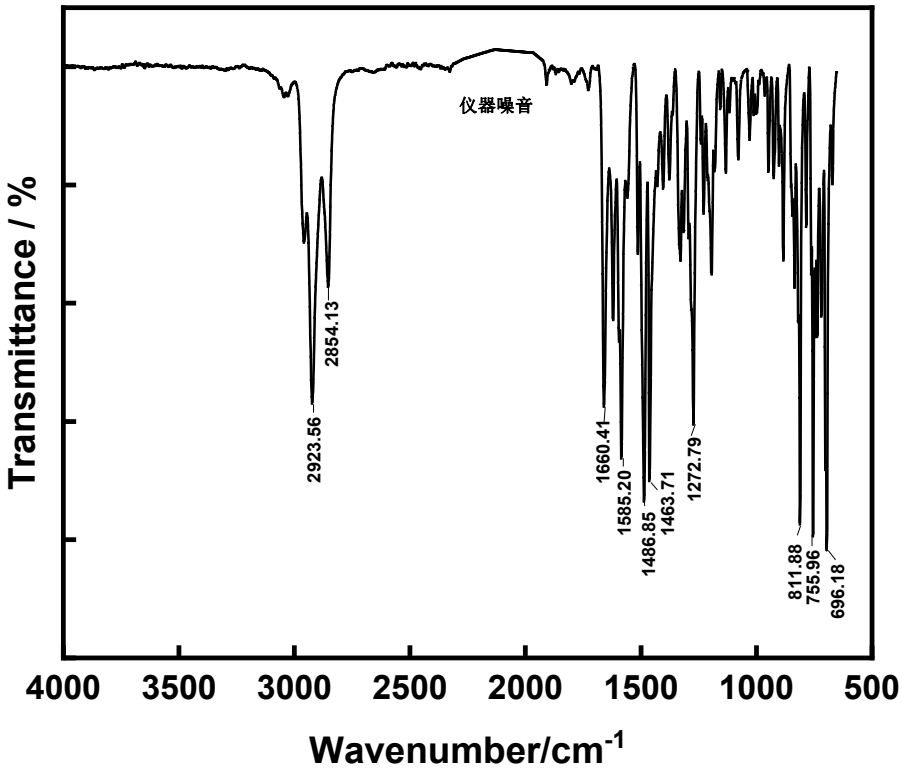


Figure S21. IR of 3b

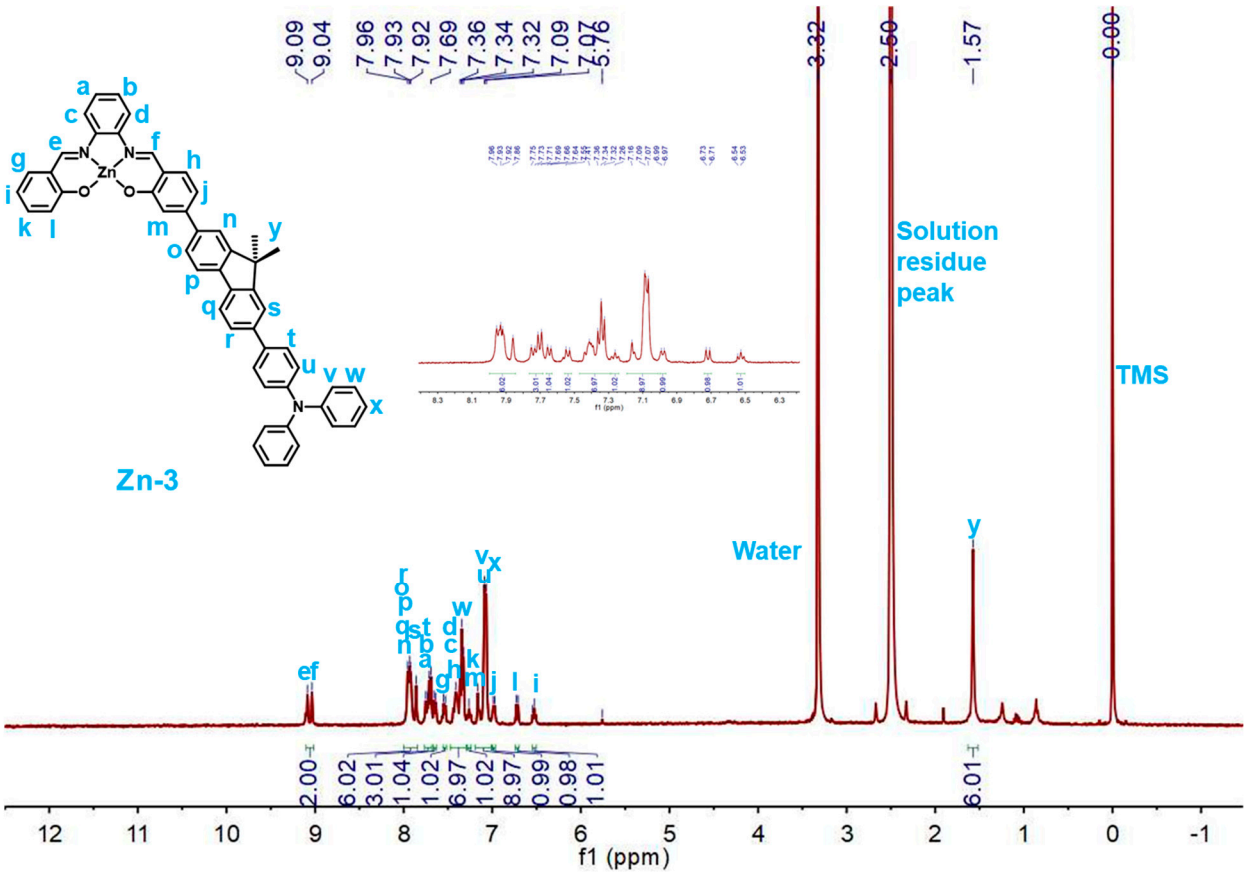


Figure S22. ^{1}H NMR of Zn-3 (400 MHz, DMSO-d$_6$)

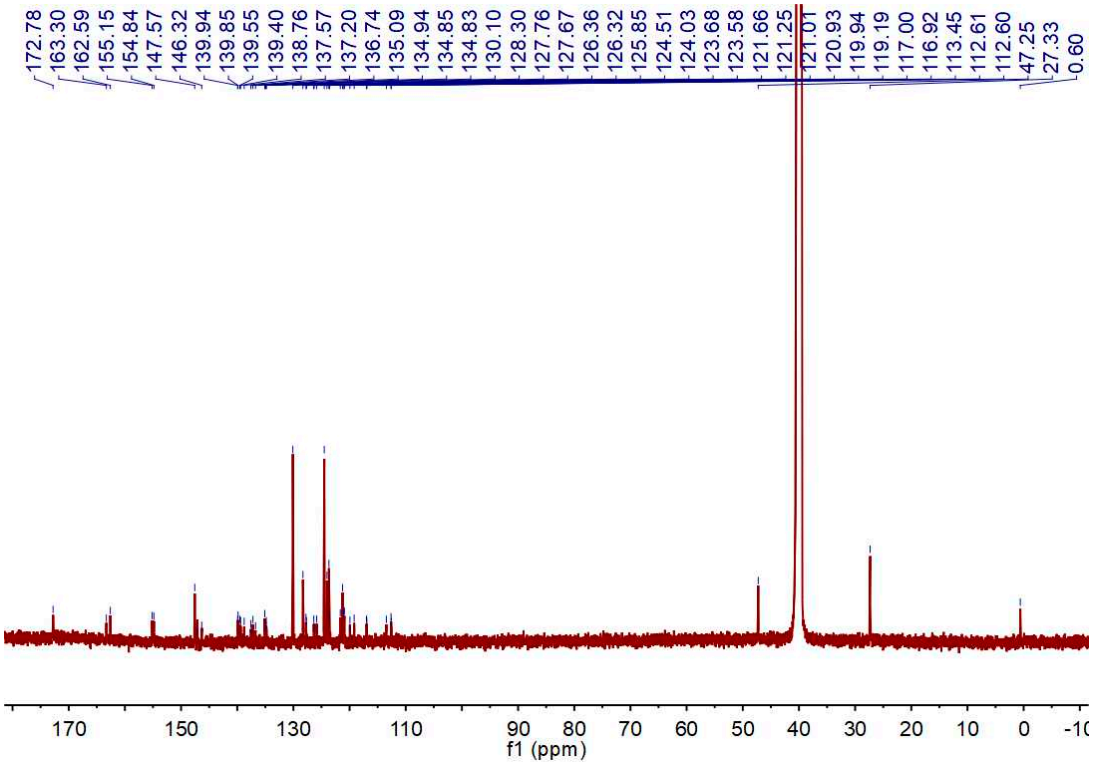


Figure S23. ^{13}C NMR of Zn-3 (600 MHz, DMSO-d$_6$)

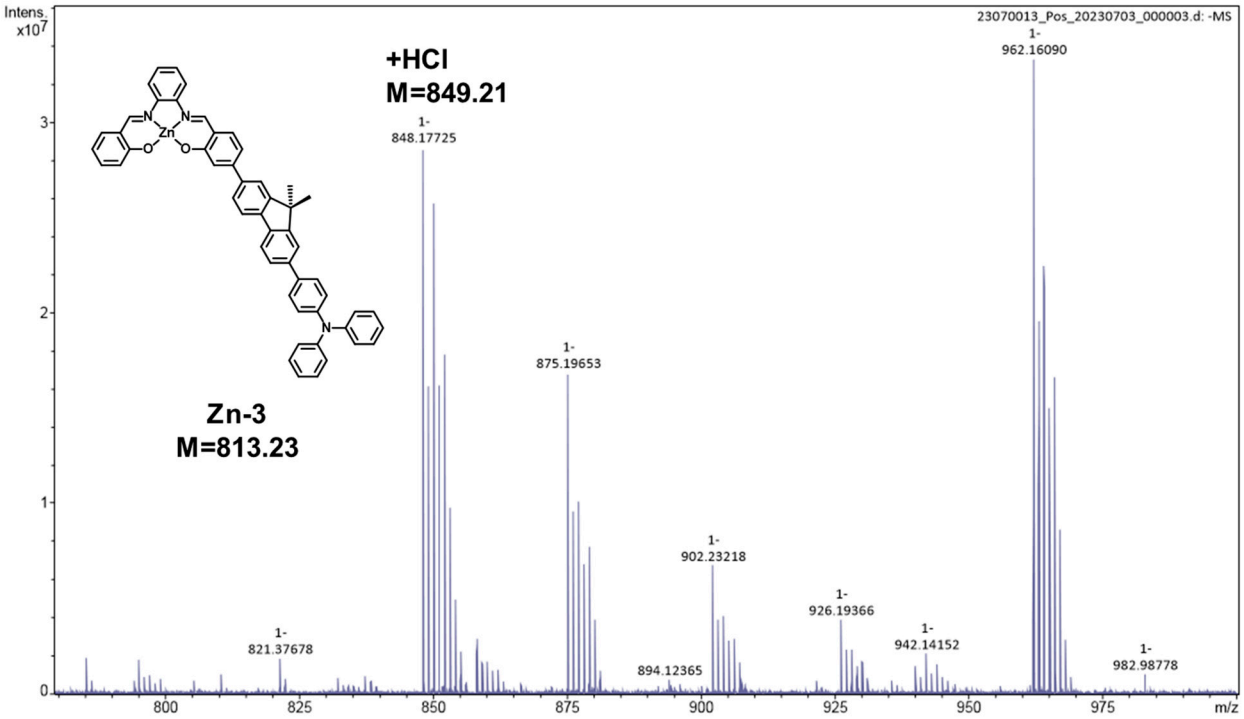


Figure S24. MS of Zn-3

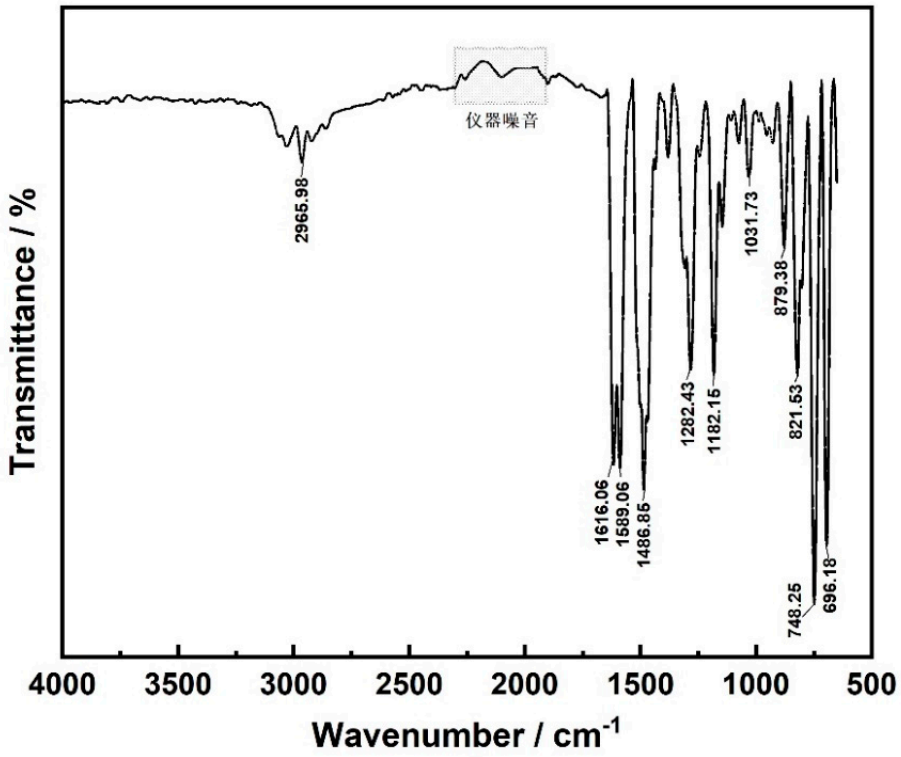


Figure S25. IR of Zn-3

4. Zn-4 and intermediate product

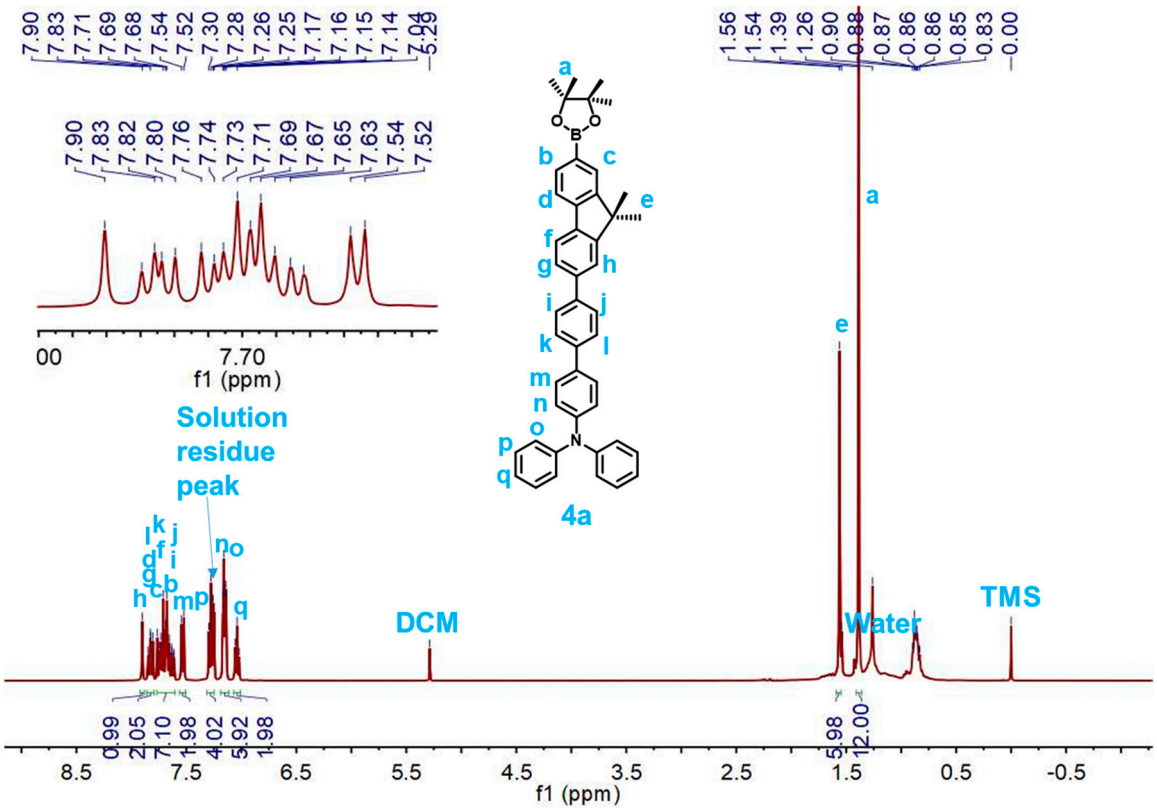


Figure S26. ^{1}H NMR of 4a (400 MHz, $CDCl_3$)

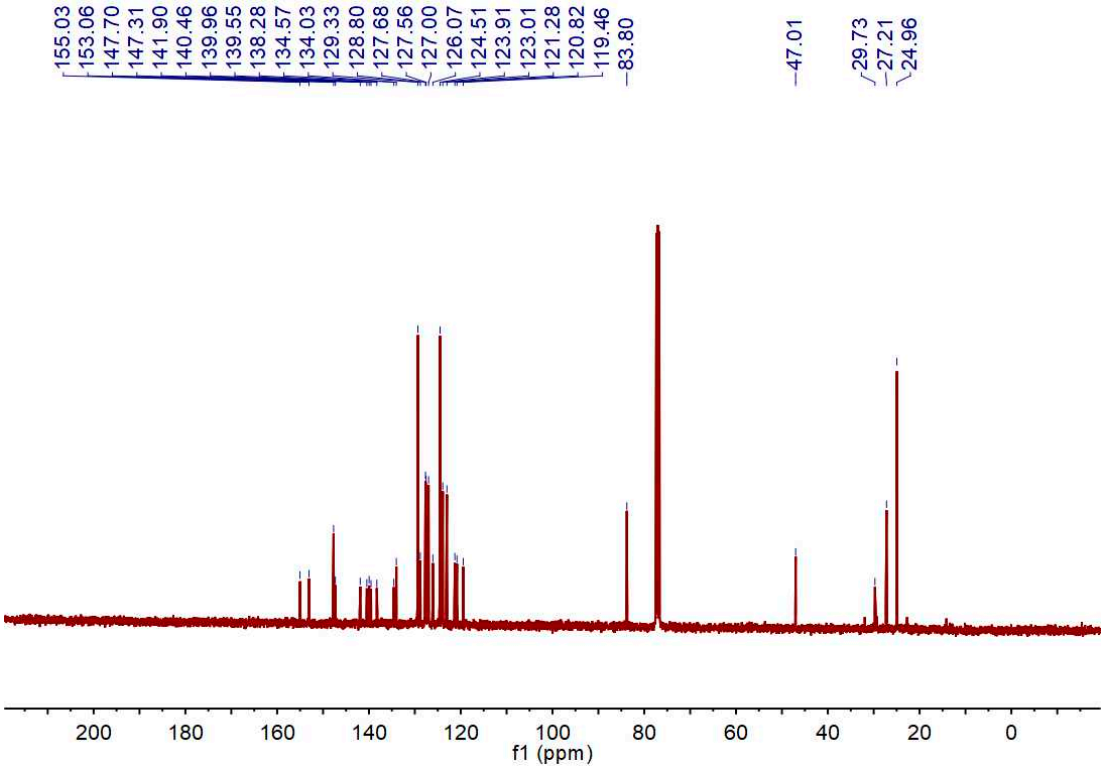


Figure S27. ^{13}C NMR of 4a (400 MHz, $CDCl_3$)

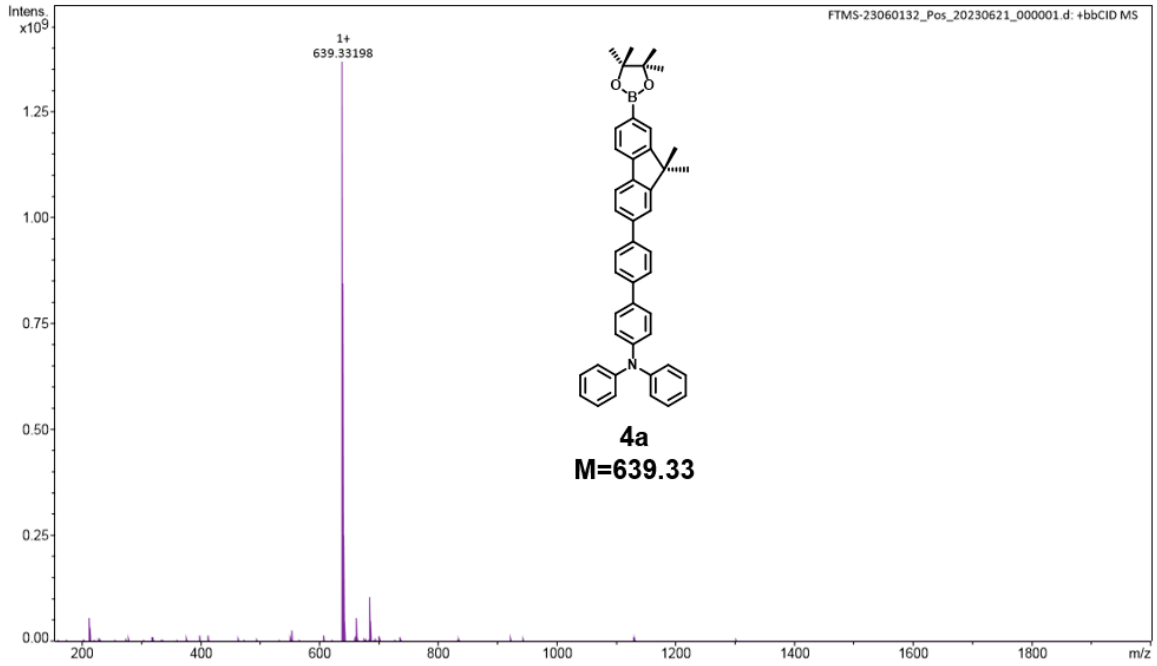


Figure S28. MS of 4a

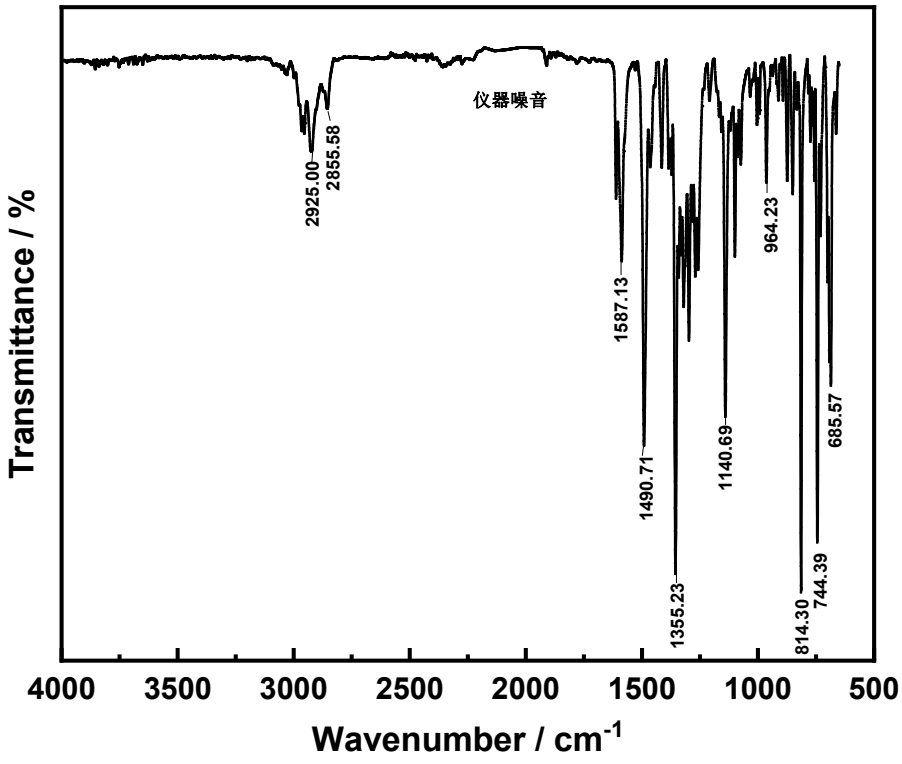


Figure S29. IR of 4a

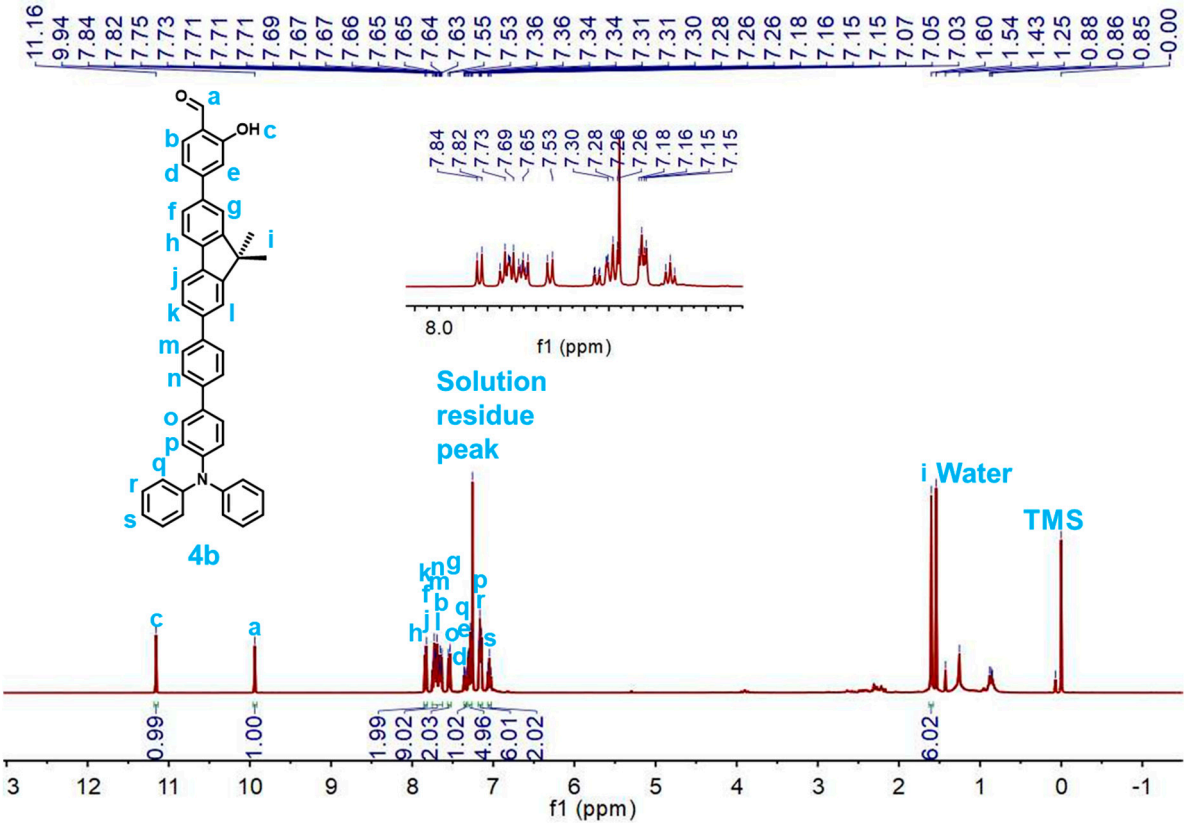


Figure S30. ^{1}H NMR of 4b (400 MHz, $CDCl_3$)

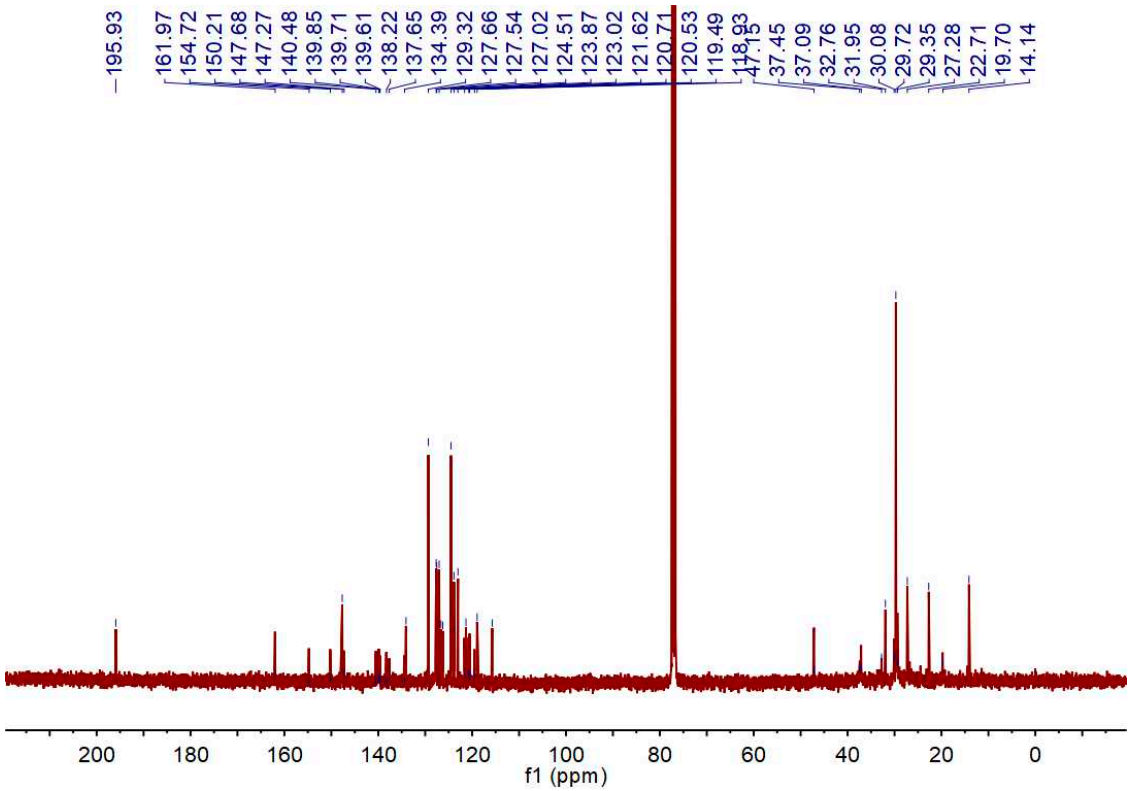


Figure S31. ^{13}C NMR of 4b (400 MHz, $CDCl_3$)

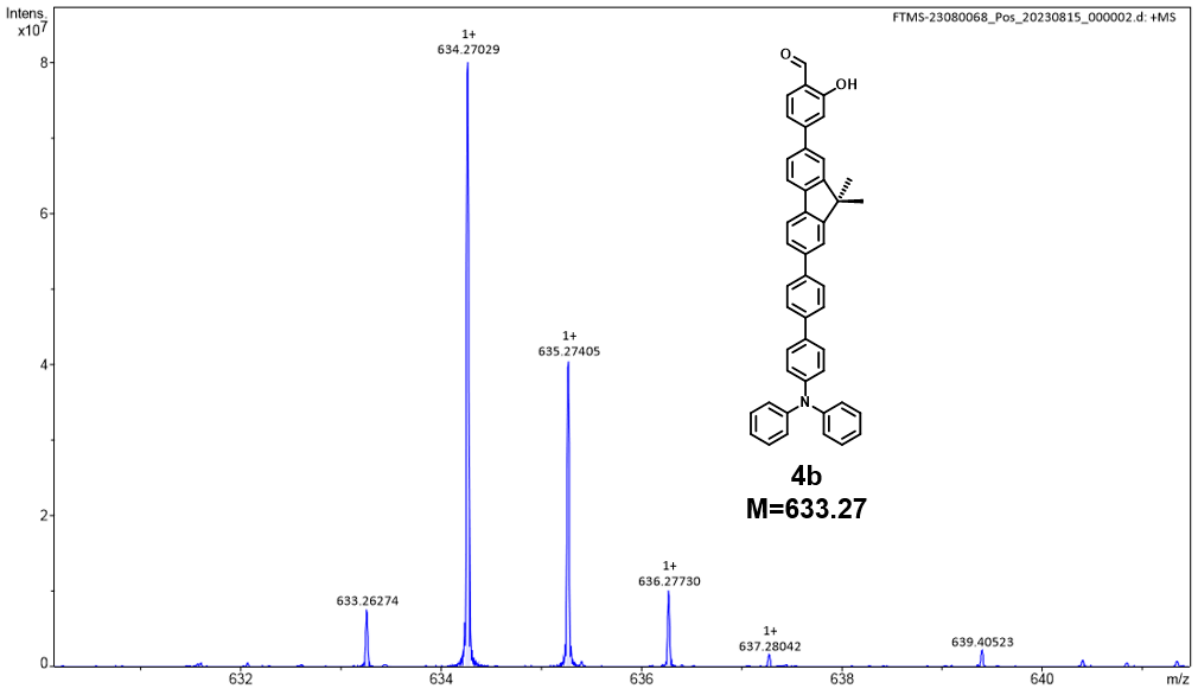


Figure S32. MS of 4b

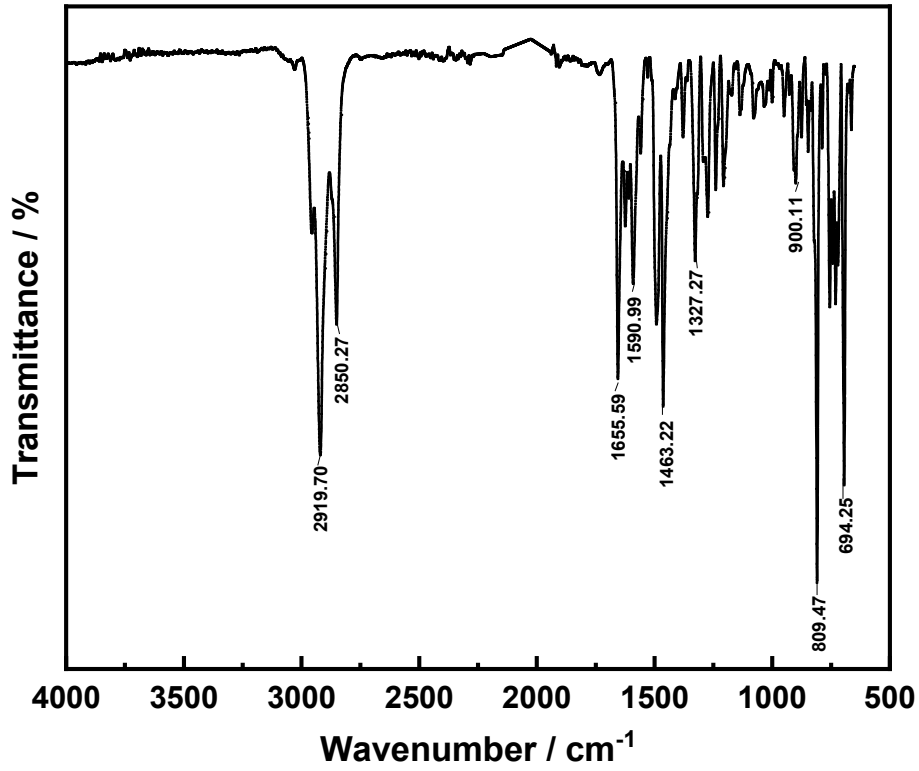


Figure S33. IR of 4b

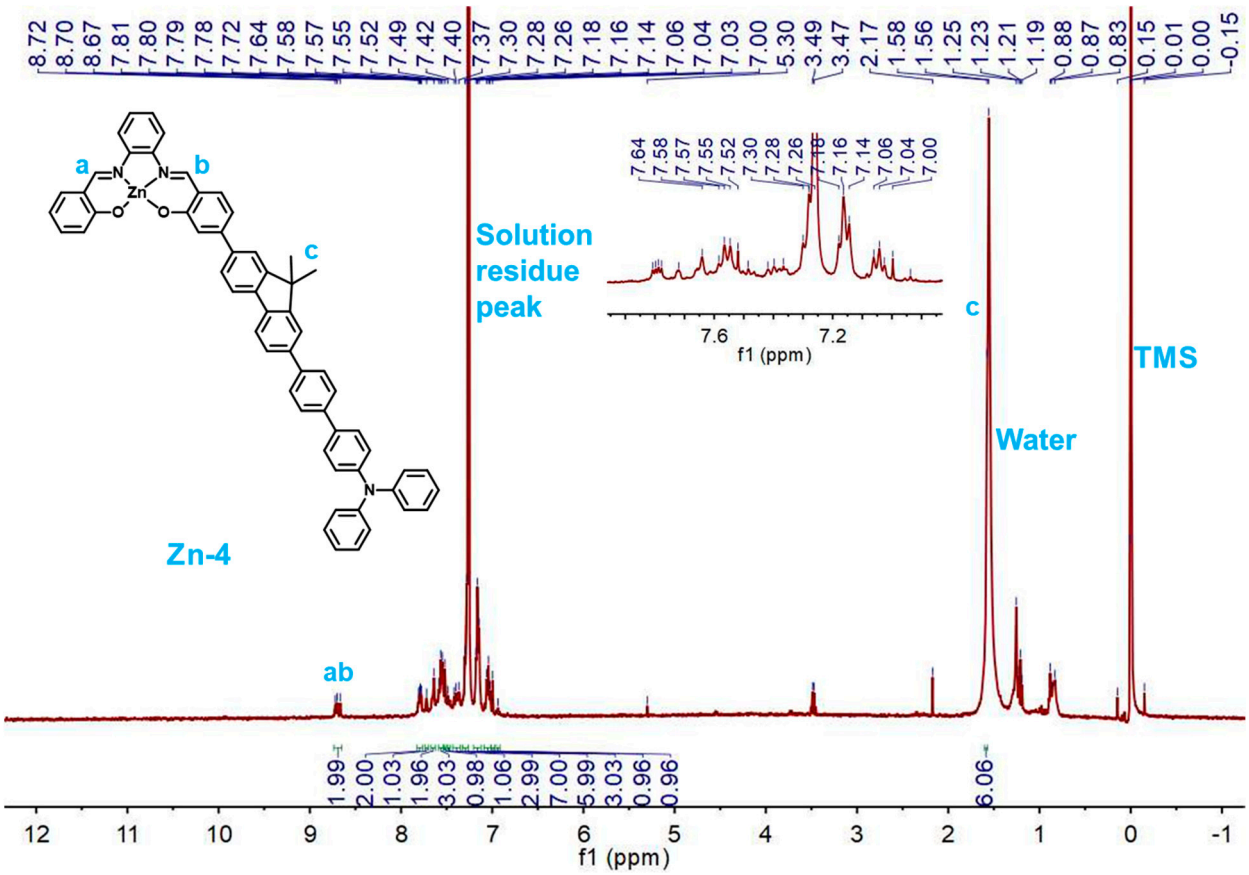


Figure S34. ^{1}H NMR of Zn-4 (400 MHz, DMSO-d$_6$)

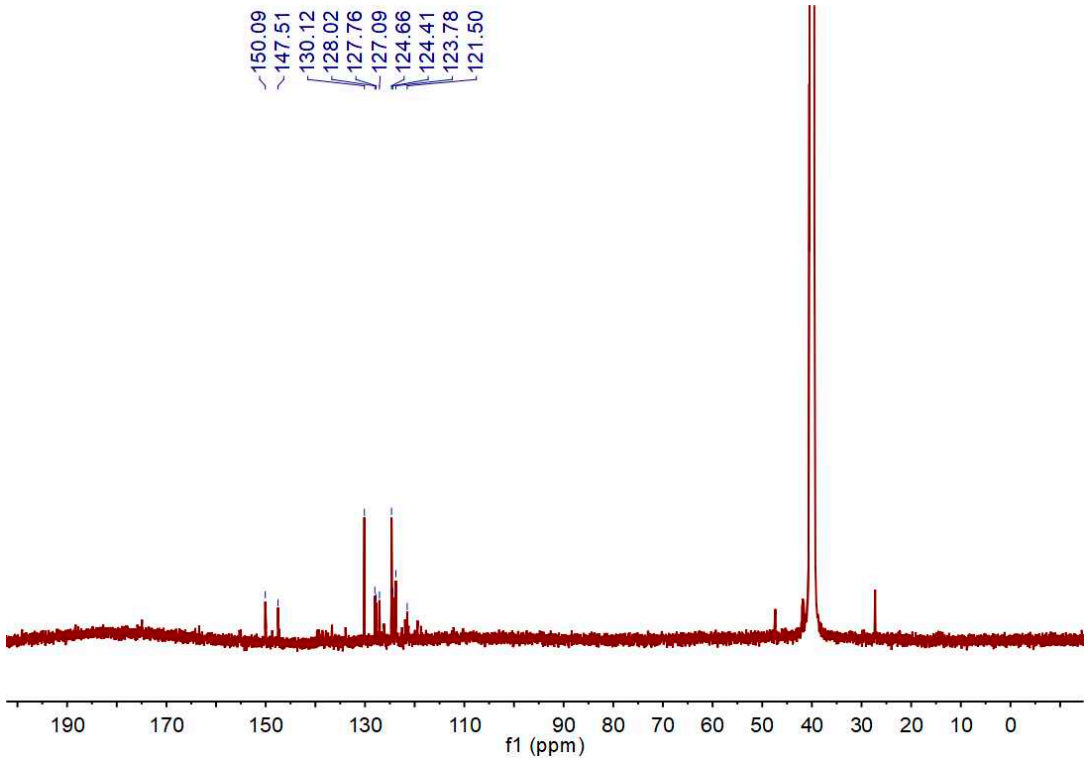


Figure S35. ^{13}C NMR of Zn-4 (600 MHz, DMSO-d$_6$)

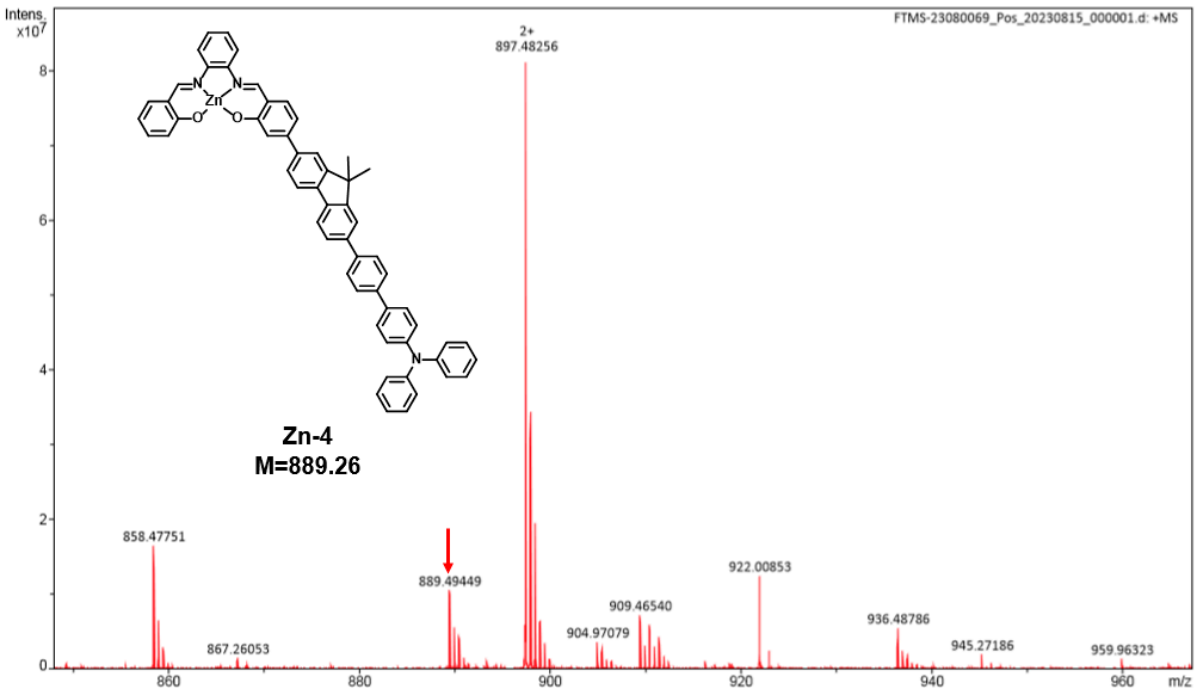


Figure S36. MS of Zn-4

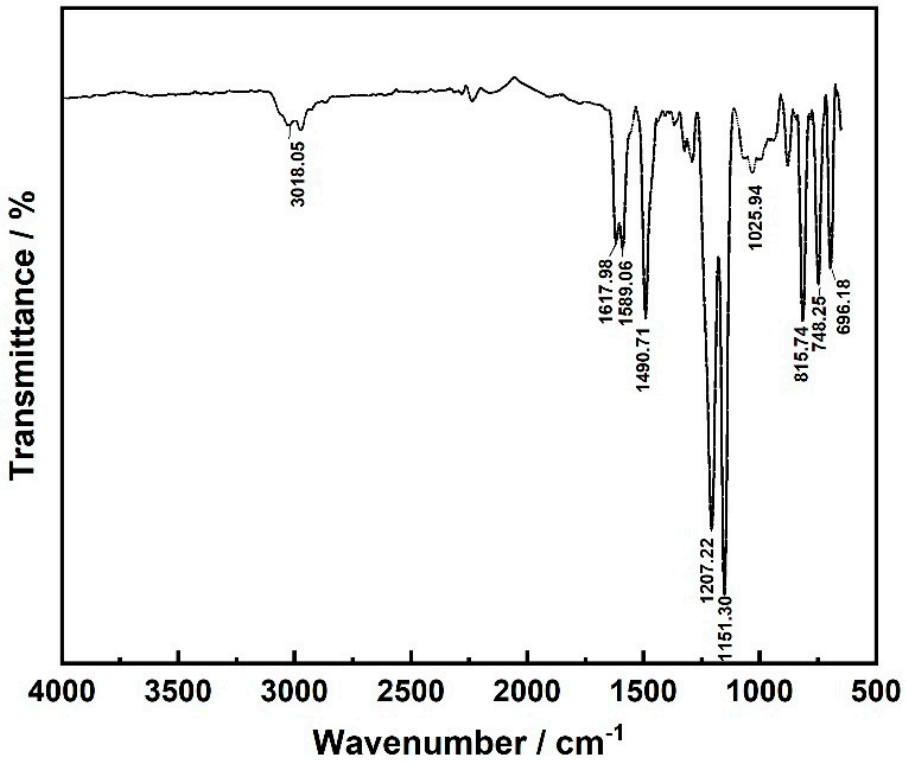


Figure S37. IR of Zn-4

Ⅱ. Extinction coefficient

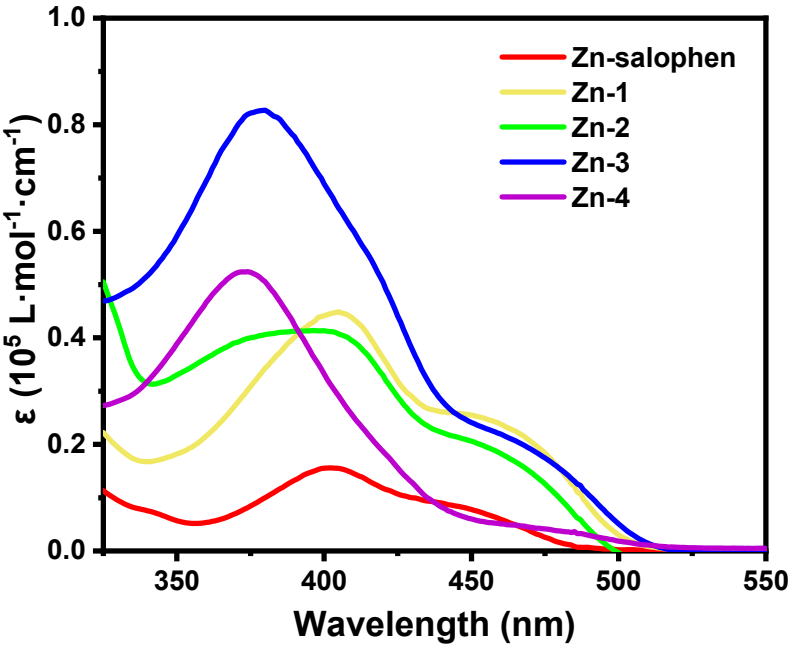


Figure S38. Extinction coefficient at absorption peaks of Zn-1-4 (Solvent: DMSO).

Table S1. Extinction coefficient of Zn-1-4 (Solvent: DMSO).

Compound	λ(nm)	logε	λ(nm)	logε
Znsalophen	405	4.19	450	3.89
Zn-1	405	4.65	455	4.39
Zn-2	405	4.61	455	4.29
Zn-3	380	4.92	455	4.36
Zn-4	375	4.72	455	3.73

Ⅲ. Fluorescence decay

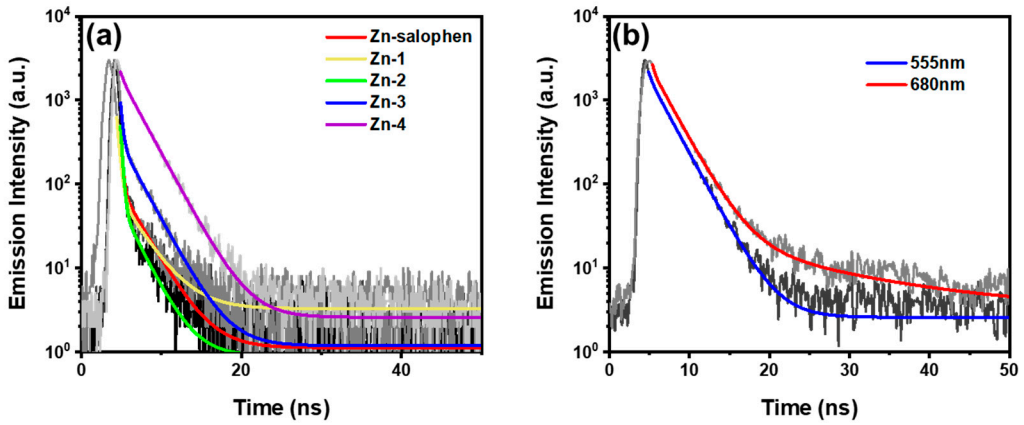


Figure S39. Fluorescence decay and fitting of Zn-1-4 (Solvent: DMSO, λ_{ex}=405 nm). (a) Comparison of fluorescence decay at emission peaks among compounds; (b) Comparison of fluorescence decay between different emission wavelengths of Zn-4

Ⅳ. lifetime of Zn-1-4 (in nitrogen)

Table S2. Fluorescence lifetime of Zn-1-4 in nitrogen condition (Solvent: DMSO, λ_{ex}=405 nm)

Compound	λ(nm)	τ(ns)(*Rel*%)	λ(nm)	τ(ns)(*Rel*%)
		0.25(37.62%)		0.33(7.51%)
Zn-salophen	520	2.56(62.38%)	650	2.15(64.00%)
				12.48(28.49%)
		0.24(36.17%)		0.28(24.16%)
Zn-1	540	2.23(63.83%)	680	2.51(54.02%)
				12.35(21.81%)
		0.26(26.33%)		0.28(23.43%)
Zn-2	540	2.18(73.67%)	680	2.29(57.26%)
				12.56(19.31%)
		0.26(16.70%)		0.33(15.48%)
Zn-3	550	2.37(83.30%)	680	2.43(73.11%)
				13.17(11.41%)
		0.39(3.54%)		0.27(2.66%)
Zn-4	555	2.44(96.46%)	680	2.45(90.54%)
				14.90(6.80%)

Ⅴ. DFT calculations

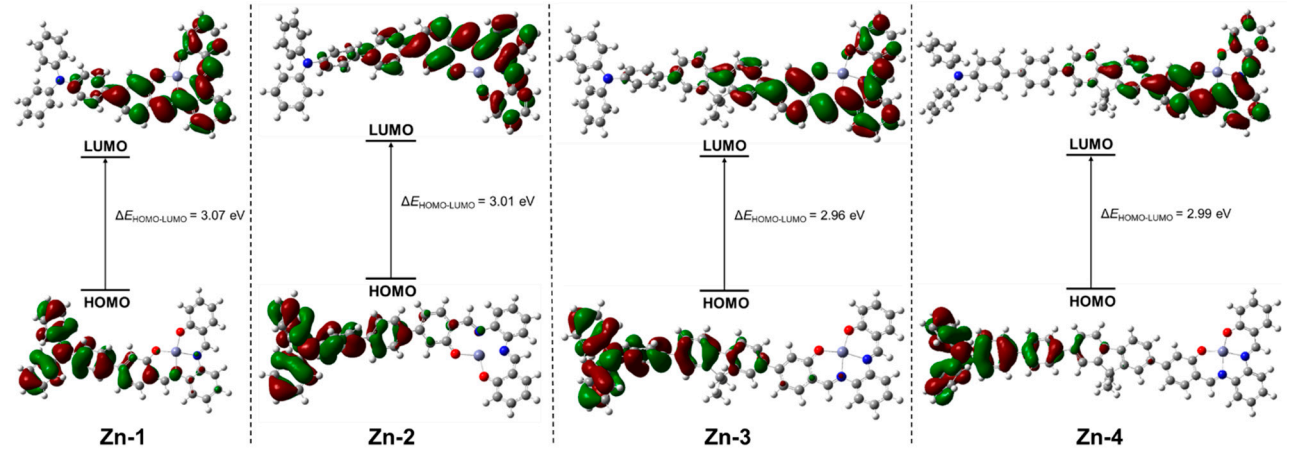


Figure S40. The frontier orbitals in ground states for **Zn-1**-**4** with HOMO-LUMO energy gaps obtained from DFT calculations (isovalue 0.02). The HOMO of each compound is predominantly localized on the triphenylamine moiety while the LUMO is mainly localized on the salophen moiety.