Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information for:

Aggregation-induced emission and reversible mechanochromic luminescence of carbazole-based triphenylacrylonitrile derivatives

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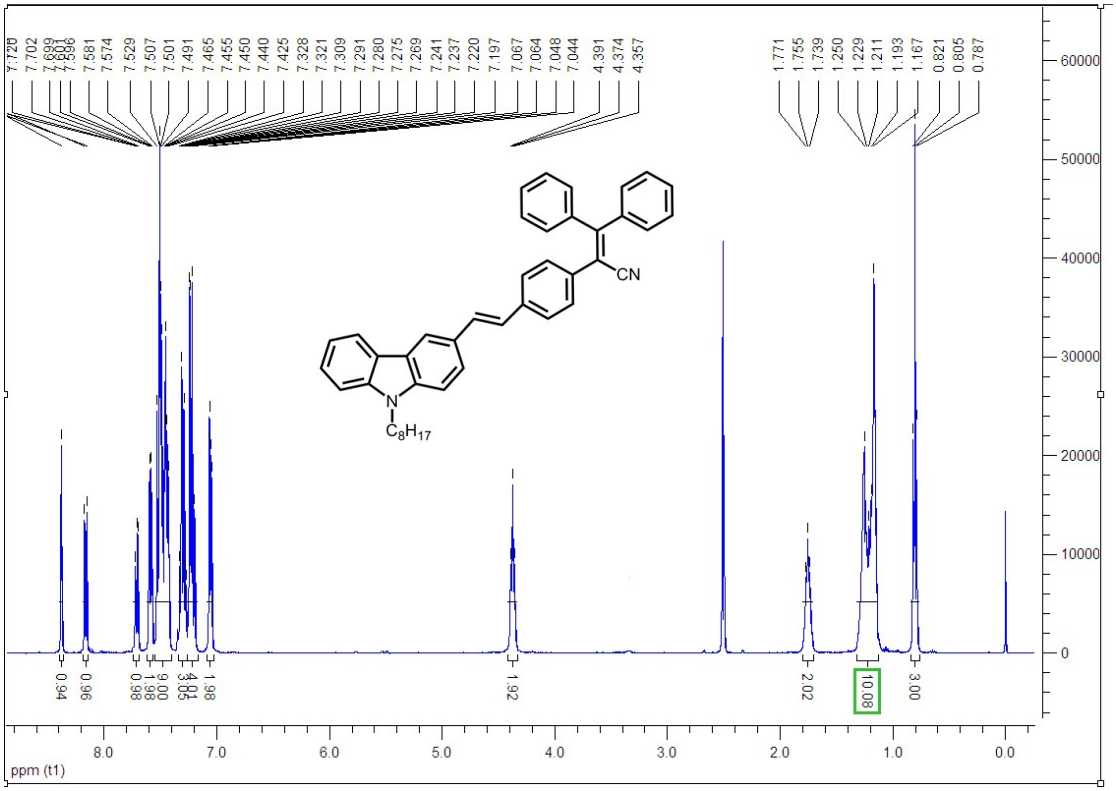
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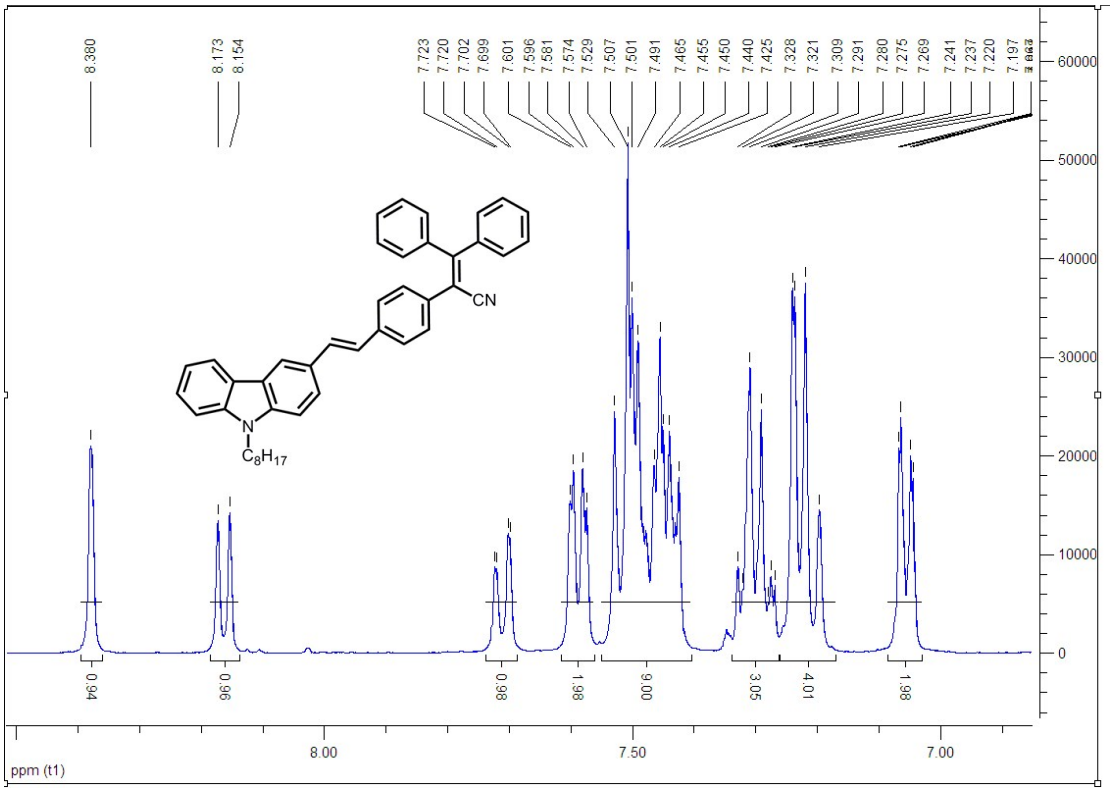
ppm (t1)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CN
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C8H17
0.94
0.96
0.98
1.98
9.00
3.05
4.01
1.98
ppm (t1)

Fig. S1 ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **Cz1-TPAN**.

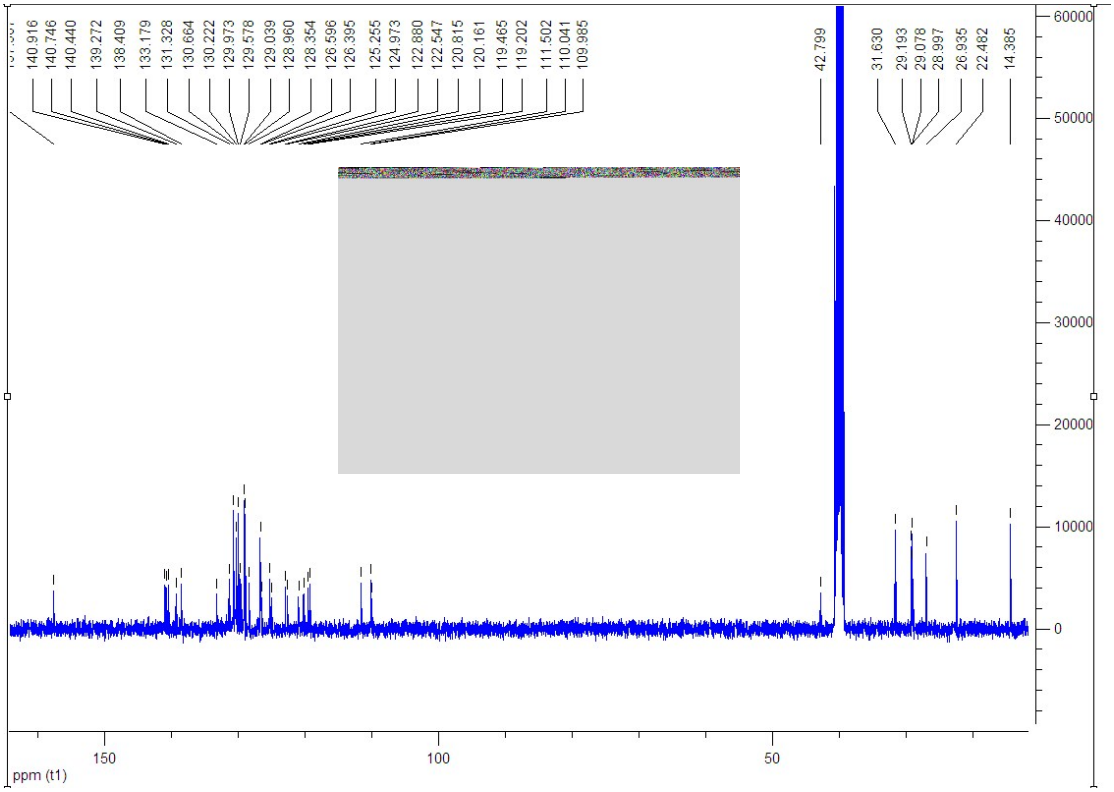


Fig. S2 ^{13}C-NMR (100 MHz, DMSO-d_6) spectrum of compound **Cz1-TPAN**.

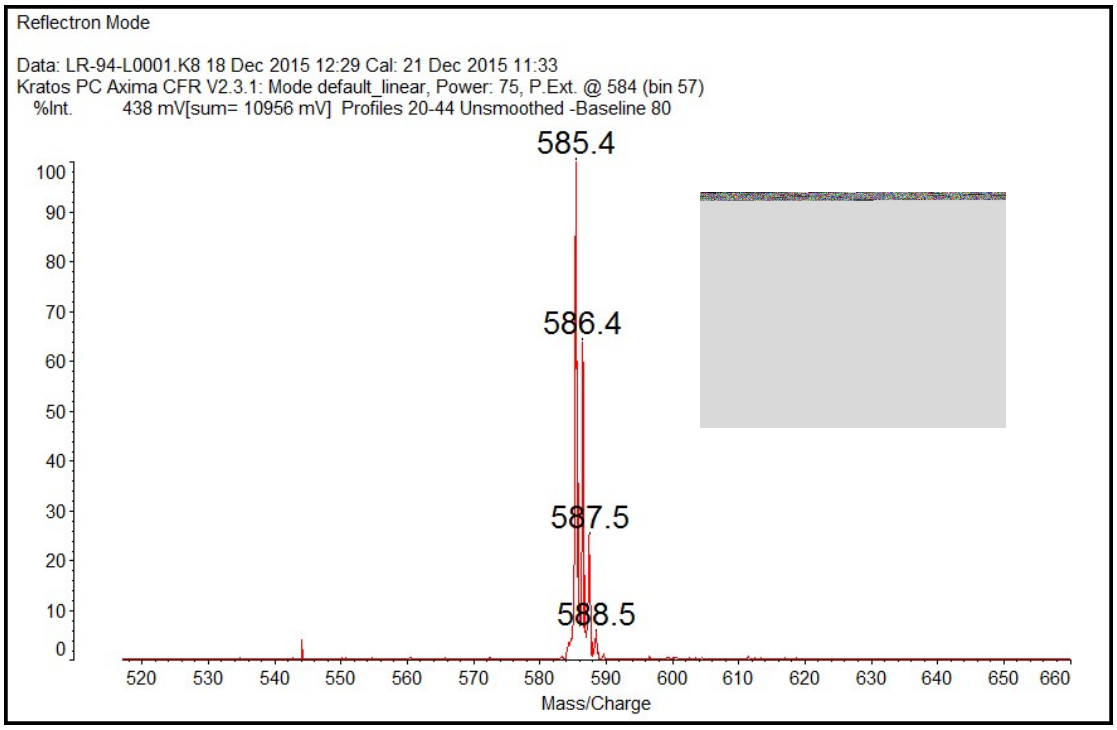


Fig. S3 The MALDI/TOF MS spectrum of compound **Cz1-TPAN**.

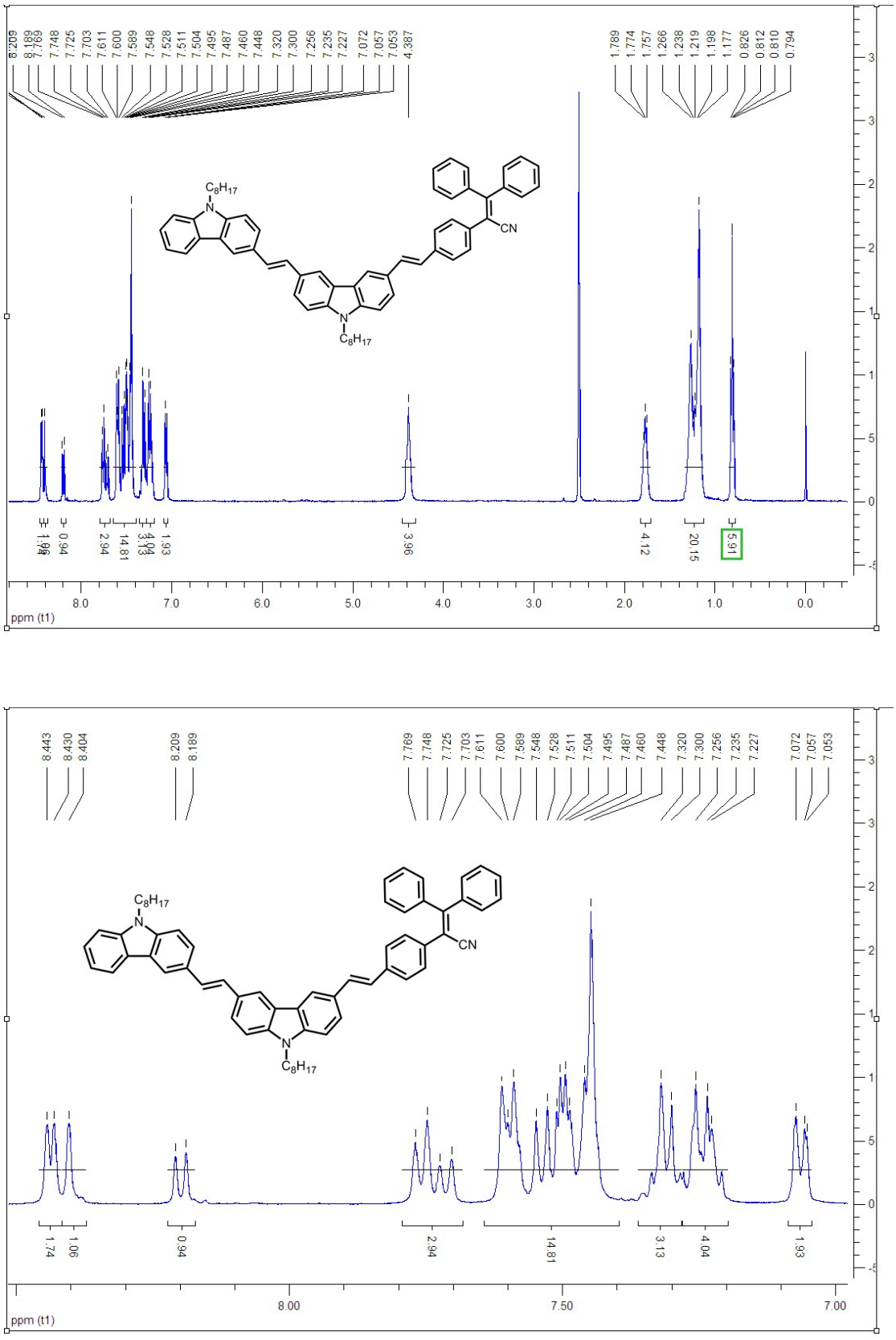


Fig. S4 ^{1}H-NMR (400 MHz, DMSO-d_6) spectra of compound **Cz2-TPAN**.

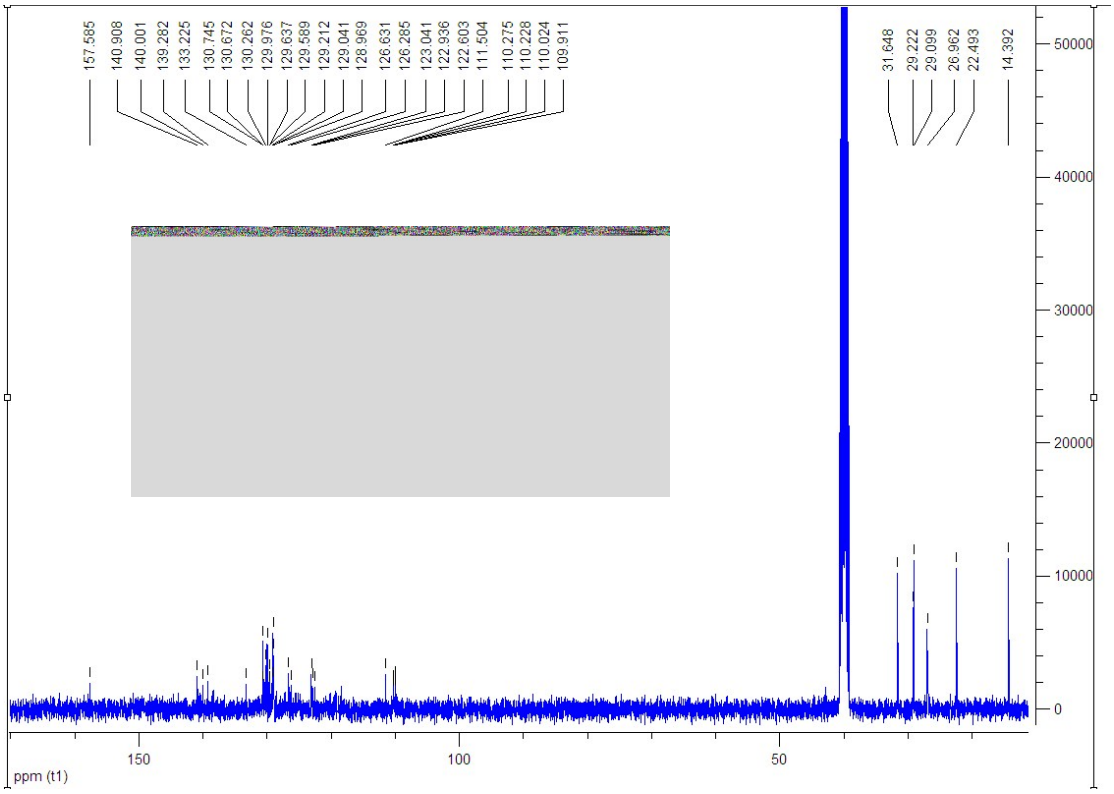


Fig. S5 ^{13}C-NMR (100 MHz, DMSO-d_6) spectrum of compound **Cz2-TPAN**.

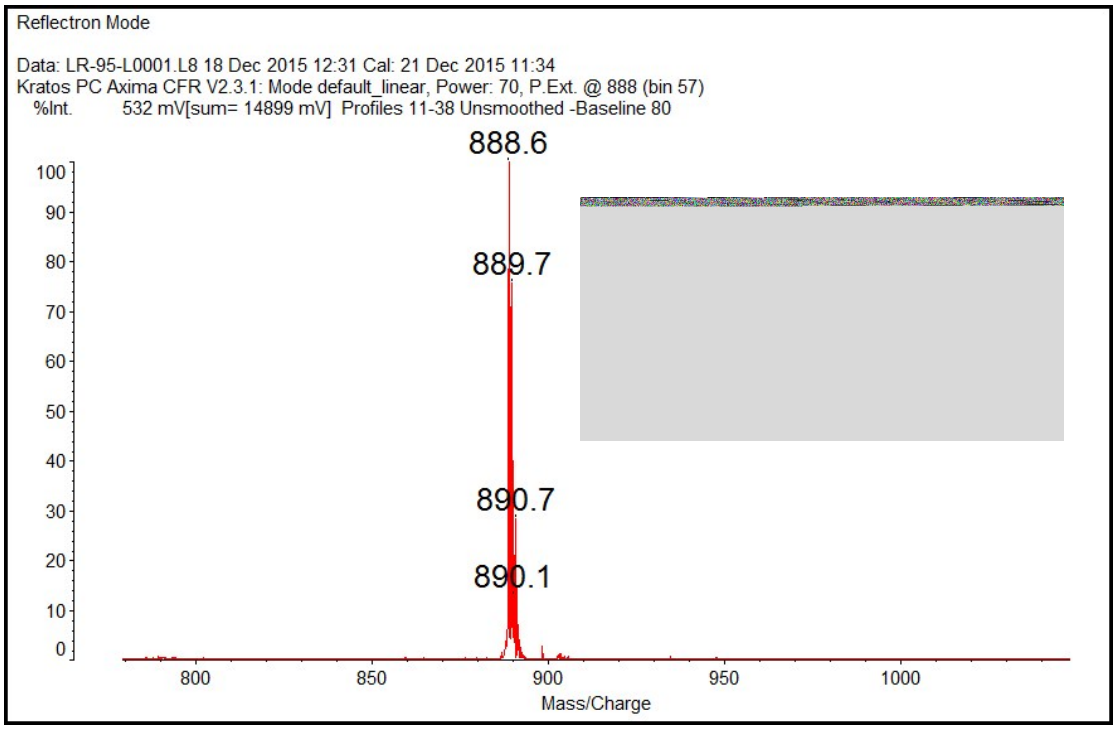


Fig. S6 The MALDI/TOF MS spectrum of compound **Cz2-TPAN**.

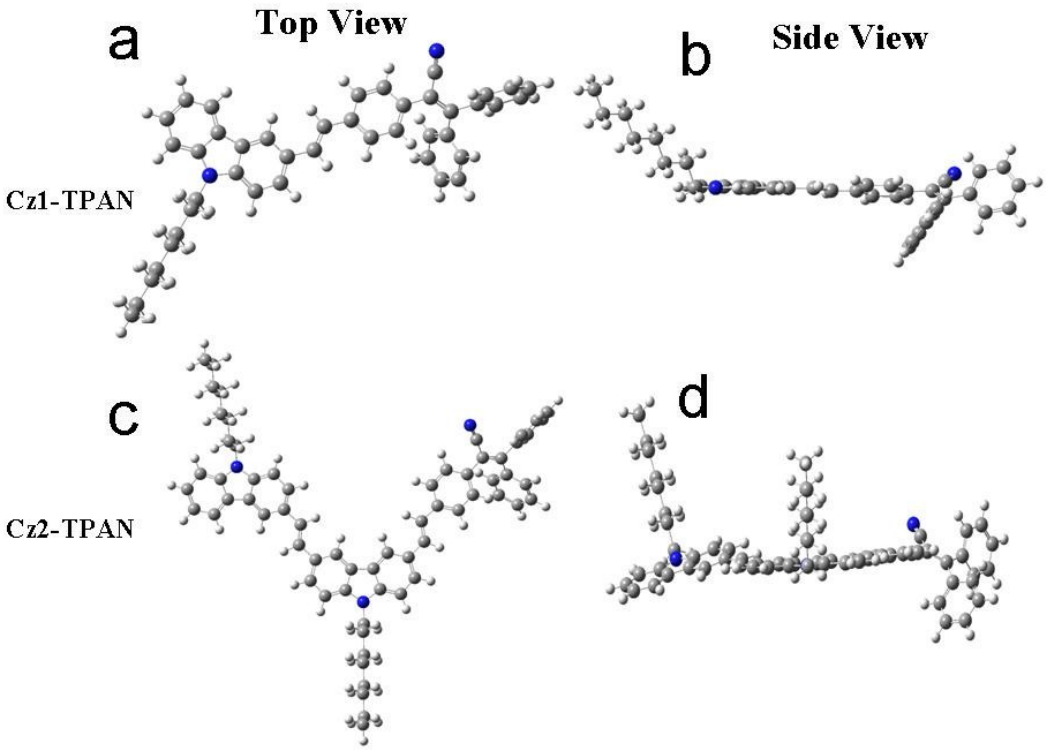


Fig. S7 The optimized molecular configurations of **Cz1-TPAN** (a, b) and **Cz2-TPAN** (c, d） in two different views calculated by the DFT method (B3LYP/6-31G level) on Gaussian 09 software.

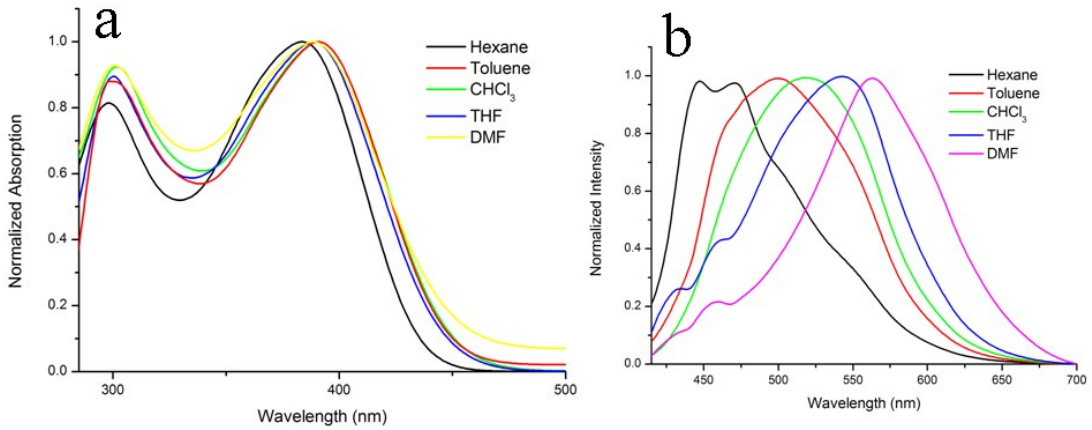


Fig. S8 Normalized UV-vis absorption (a) and fluorescence emission (b, λ_{ex} = 400 nm) spectra of **Cz1-TPAN** in different solvents (2.0 × 10^{-5} M).

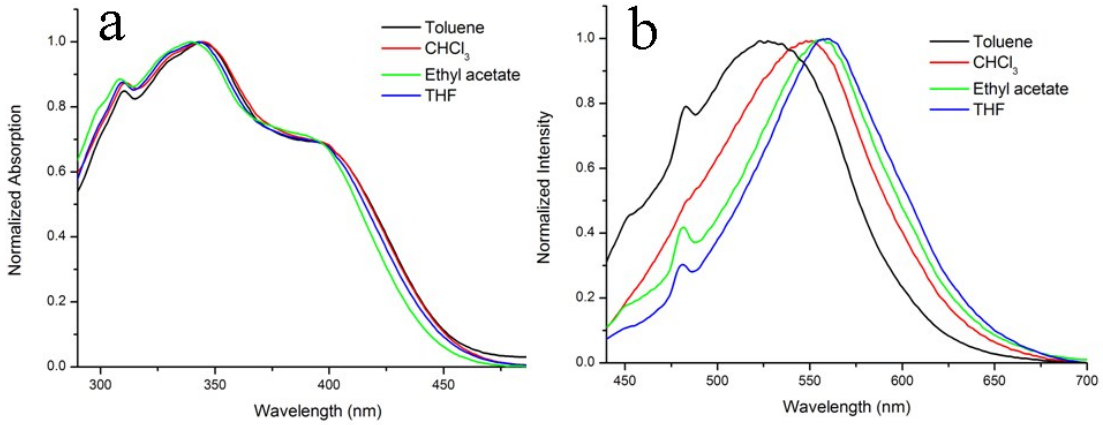
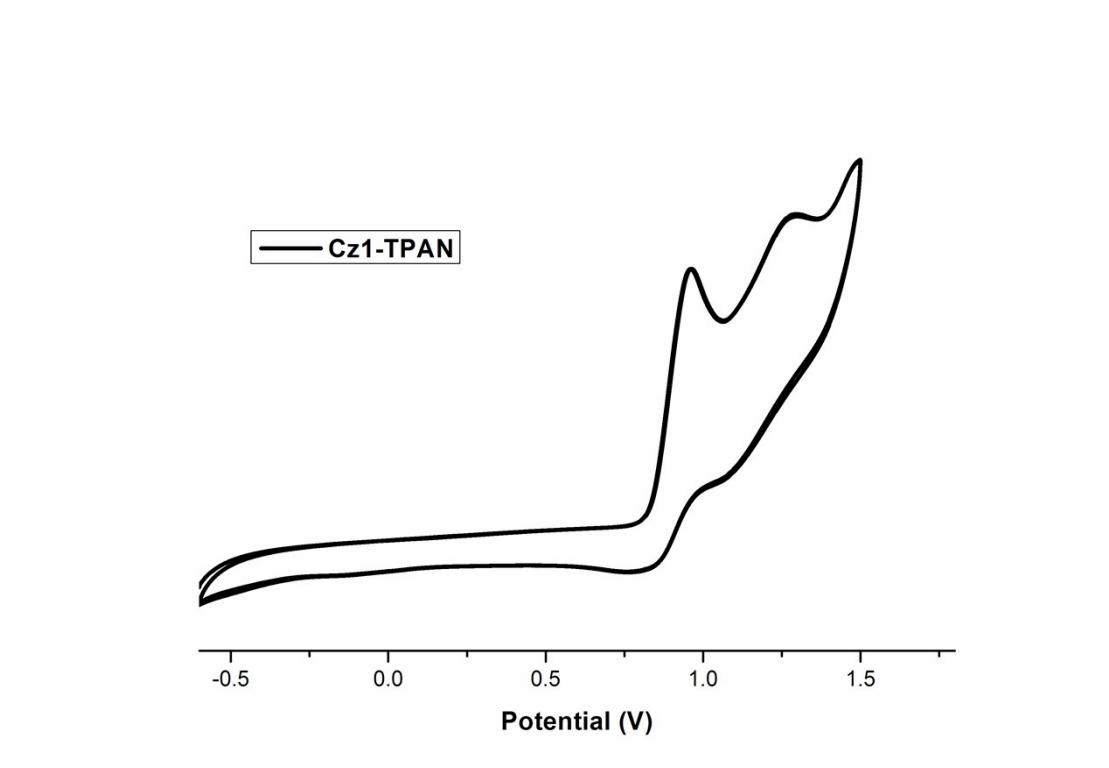


Fig. S9 Normalized UV-vis absorption (a) and fluorescence emission (b, λ_{ex} = 420 nm) spectra of **Cz2-TPAN** in different solvents (2.0 × 10^{-5} M).



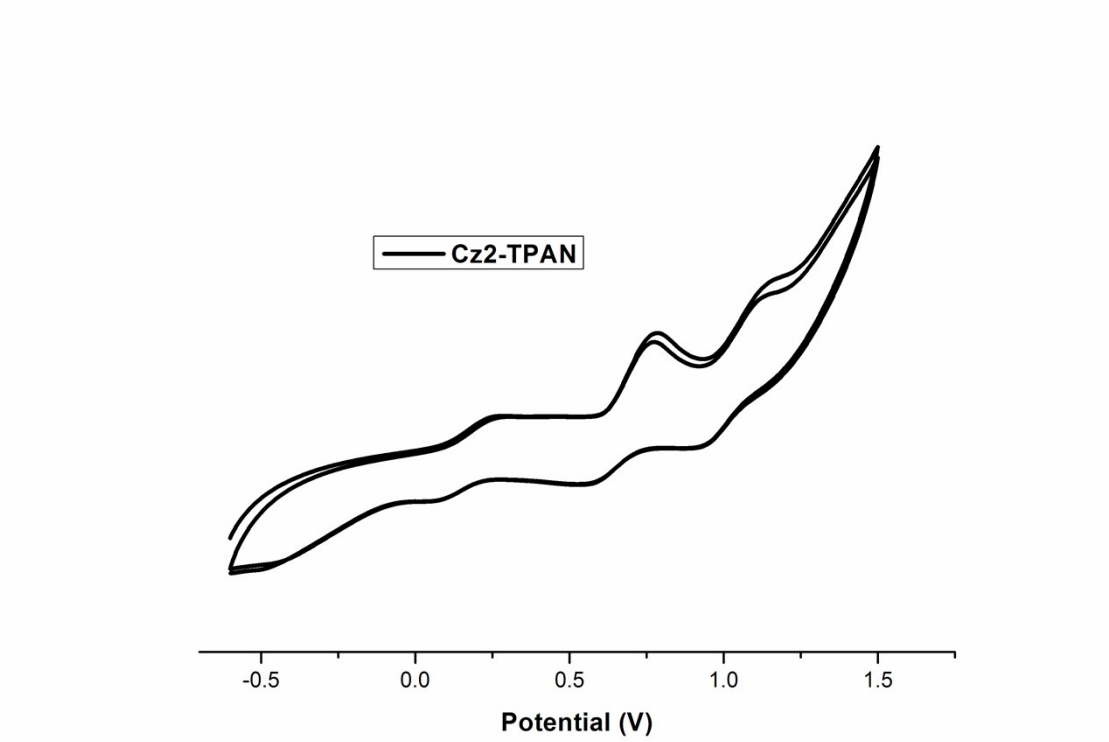


Fig. S10 Cyclic voltammetry diagrams of **Cz1-TPAN** and **Cz2-TPAN** in anhydrous CH_2Cl_2 with 0.1 M Bu_4NPF_6 as electrolyte at a scan rate of 50 mV/s.

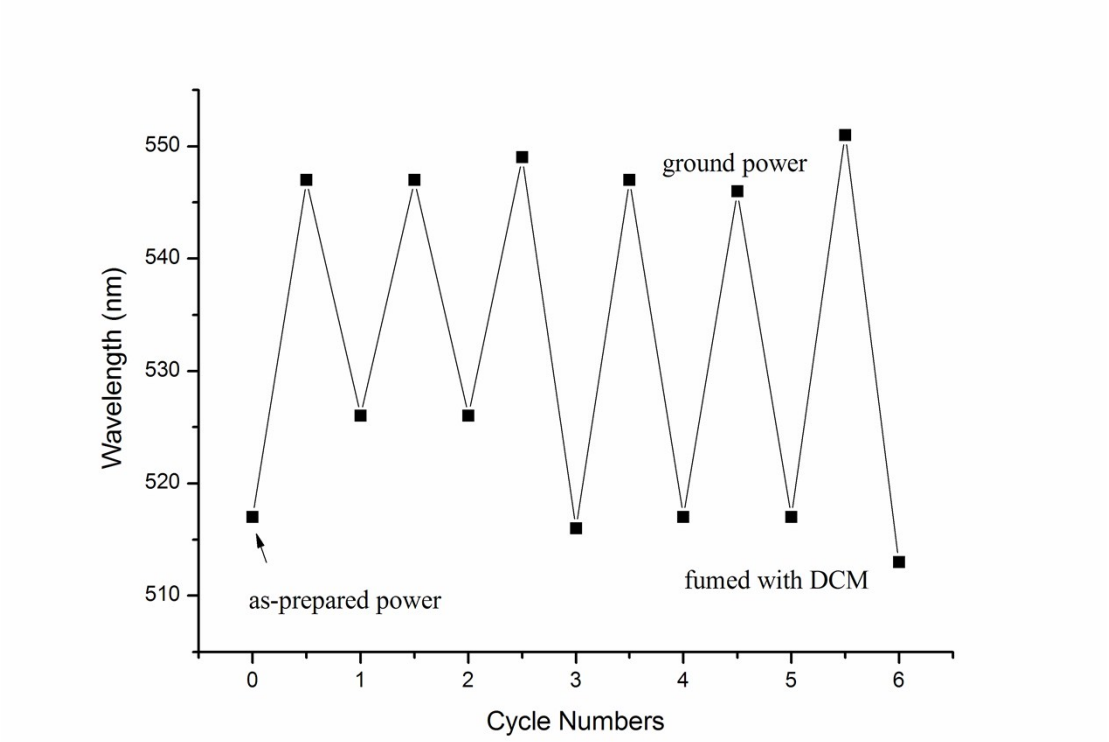


Fig. S11 Maximum fluorescent emission of **Cz1-TPAN** upon repeating treatment of grinding and fuming with DCM.

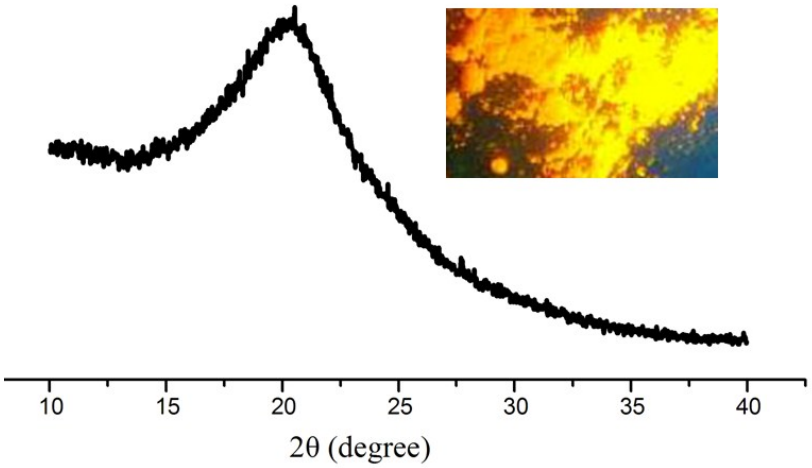


Fig. S12 XRD patterns of **Cz2-TPAN** in as-synthesized solid states. Inset is photographs in as-synthesized solid states under UV illumination.

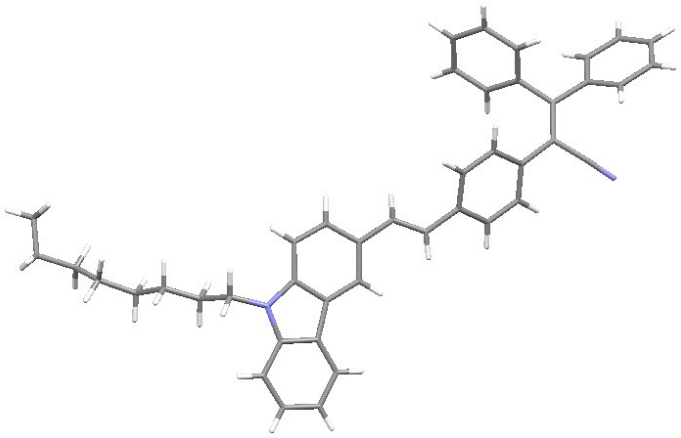


Fig. S13 The structure of **Cz1-TPAN** in single crystal.

Table S1 Electrochemical data and HOMO/LUMO energy levels of **Cz1-TPAN** and **Cz2-TPAN**.

Compounds	$E_{1/2}^{oxa}$ (V)	HOMO[b] (eV)	LUMO[b] (eV)	E_g[c] (eV)	HOMO[d] (eV)	LUMO[d] (eV)
Cz1-TPAN	0.88	–5.29	–2.51	2.78	–5.02	–1.94
Cz2-TPAN	0.68	–5.09	–2.35	2.74	–4.71	–1.94

[a] $E_{1/2}^{ox}$ = first half-wave potential; Fc/ Fc^+ was used as the external reference. [b] calculated using the empirical equation: $E_{HOMO} = -(E_{1/2}^{ox} + 4.41)$ and $E_{LUMO} = E_{HOMO} + E_g$. [c] Estimated from the onset of the absorption spectra ($E_g = 1240/\lambda_{onset}$). [d] Obtained from quantum chemical calculation using TDDFT/B3LYP/ 6-31G(d).